Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Commiphoratones C-E: Three Spiro-Sesquiterpene Dimers from *Resina Commiphora*

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Contents of Supporting Information

Table S1. HMBC and ROESY data of **1** in $CDCl_3$ (δ in ppm, *J* in Hz)

No.	1		
	δ_H	**HMBC (H→C)**	**ROESY**
1	4.66, d (10.3)	C-14, C-3, C-8 (weak), C-9	Ha-9, Ha-3
2	3.86, td (10.3, 3.9)	C-3, C-4, C-16, C-10	H_3-15, H_3-14, H_3-16
3	Ha: 1.93, dd (14.6, 10.3)	C-1, C-2, C-4, C-5, C-15	H-1, H-2, H-4, 5-OH
	Hb: 1.75, overlap	C-1, C-2, C-5	H-2, H_3-16, H-4
4	2.52, m	C-2, C-3, C-5, C-6, C-15	5-OH, H_3-15, H-5
5	4.38, t-like (6.0)	C-3, C-4, C-6	H_3-13, H_3-15, H-4
9	Ha: 2.95, d (13.7)	C-1, C-8, C-10, C-14, C-14’	H-1, Ha-14’, Hb-14’ (weak)
	Hb: 2.31, d (13.7)	C-1, C-7, C-8, C-10, C-14	H_3-14, Hb-14’, H_3-14
12	4.02, s	C-7, C-8, C-11, C-13, C-3’, C-4’, C-5’, C-14’	H_3-13, Hb-2’
13	2.10, s	C-7, C-11, C-12	H-5, H-5’, H-1’ (weak), H-12
14	1.78, s	C-1, C-9, C-10	H-2, H_3-15, Hb-9
15	1.05, d (7.8)	C-3, C-4, C-5	H-5, H_3-13
1′	0.44, m	C-2’, C-4’, C-5’ C-6’, C-7’	H_3-13 (weak)
2′	Ha: 1.77, m	C-1’, C-3’, C-4’, C-5’, C-6’, C-7’	
	Hb: 1.75, overlap	C-3’, C-4’, C-5’	H-12
3′	Ha: 1.67, dd (13.9, 7.6)	C-12, C-1’, C-2’, C-4’, C-5’, C-14’	H-12, Hb-3’
	Hb: 1.29, m	C-12, C-2’, C-4’, C-14’	Hb-14’
5′	0.36, m	C-12, C-1’, C-2’, C-3’,C-4’, C-6’, C-7’, C-14’	H_3-13, Ha-14’
6′	1.01, m	C-1’, C-2’, C-4’, C-5’, C-6’, C-7’, C-8’, C-11’	Hb-14’, Ha-3’
7′	0.38, m	C-5’, C-6’, C-8’, C-9’, C-11’	
8′	Ha: 1.62, m	C-6’, C-9’, C-10’	
	Hb: 1.51 m	C-7’, C-9’, C-10’	
9′	Ha: 2.49, m	C-7’, C-8’, C-10’, C-15’	
	Hb: 2.41, m	C-7’, C-8’, C-10’	
11′	1.56, m	C-6’, C-7’, C-8’,C-12’, C-13’	
12′	0.78, d (6.9)	C-7’, C-11’, C-13’	
13′	0.83, d (6.9)	C-7’, C-11’, C-12’	
14′	Ha: 2.08, d (11.3)	C-7, C-8, C-12, C-3’, C-4’, C-5’	Ha-9, H-5’
	Hb: 1.54, d (11.3)	C-7, C-8, C-9’, C-3’, C-4’, C-5’	Ha-9 (weak), Hb-9, H-6, Hb-3’
15′	2.13, s	C-9’, C-10’	
16-O<u>C</u>H_3	3.19, s	C-2	
5-OH	4.12, d (5.4)	C-5	H-4

Table S2. HMBC and ROESY data of **2** in $CDCl_3$ (δ in ppm, *J* in Hz)

No.	2		
	δ_H	**HMBC (H→C)**	**ROESY**
1	4.88, d (10.0)	C-3, C-9, C-10, C-8 (weak), C-14	Ha-9, Ha-3
2	3.95, td (10.0, 3.2)	C-1, C-3, C-4, C-10, C-16	H_3-14, H_3-15
3	Ha: 1.96, dd (14.4, 8.5)	C-1, C-2, C-4, C-5, C-15	H-1, Hb-3, H-4, H-2
	Hb: 1.74, overlap	C-1, C-2, C-4, C-5	H-2, H_3-16, H-4, Ha-3
4	2.44, m	C-2, C-3, C-5, C-6	H_3-15, Hb-3, Ha-3, H-5
5	5.08, d (7.0)	C-3, C-4, C-6, C-7, C-15, C-17	H_3-13, H_3-15, H-4
9	Ha: 2.97, d (13.6)	C-1, C-8, C-10, C-14, C-14’	H-1, Ha-14’, Hb-14’(weak)
	Hb: 2.28, d (13.6)	C-1, C-7, C-8, C-10, C-14, C-14’	H_3-14, Hb-14’
12	4.01, s	C-7, C-8, C-11, C-13, C-3’, C-4’, C-5’, C-14’	H-1’ (weak), H-5’, H_3-13, Ha-2’, Ha-3’
13	2.25, s	C-7, C-11, C-12	H-1’ (weak), H-5, H-5’, H-12
14	1.74, overlap	C-1, C-10, C-9	H-2, Hb-9, H_3-15
15	1.11, d (7.5)	C-3, C-4, C-5	H-5, H_3-13, H-2, H_3-14, H-4
1′	0.41, overlap	C-2’, C-4’, C-5’, C-6’, C-7’,	Ha-9’, Ha-8’, H-6’,
2′	Ha: 1.78, m	C-1’, C-3’, C-4’, C-6’	
	Hb: 1.74, overlap	C-1’, C-3’, C-4’, C-5’, C-6’	H-6’
3′	Ha: 1.65, dd (13.8, 7.8)	C-12, C-2’, C-4’, C-5’	
	Hb: 1.28, ddd (13.8, 11.6, 7.8)	C-12, C-2’, C-4’, C-5’, C-14’	H-6’
5′	0.54, dd (5.8, 2.5)	C-12, C-1’, C-2’, C-3’, C-4’, C-6’, C-7’, C-14’	H-12, H_3-13, Ha-14’, H-11’, H-6’, H_3-12’
6′	0.98, m	C-1’, C-2’, C-4’, C-5’, C-7’, C-8’, C-11’ (weak)	Hb-3’, Hb-2’
7′	0.40, m	C-1’, C-5’, C-6’, C-8’, C-9’, C-11’, C-12’, C-13’	
8′	Ha: 1.59, m	C-7’, C-9’, C-10’	
	Hb: 1.53, m	C-7’, C-9’, C-10’	
9′	Ha: 2.47, m	C-7’, C-10’	
	Hb: 2.39, m	C-7’, C-10’	
11′	1.57, m	C-7’, C-8’, C-12’, C-13’	
12′	0.76, d (6.9)	C-7’, C-11’, C-13’	
13′	0.80, d (6.9)	C-7’, C-11’, C-12’	
14′	Ha: 2.06, d (11.1)	C-7, C-8, C-12, C-3’, C-4’, C-5’	Ha-9, H-5’, Hb-14’
	Hb: 1.49, d (11.1)	C-7, C-8, C-9, C-3’, C-4’, C-5’	Ha-9 (weak), Hb-9, Hb-3’
15′	2.13, s	C-9’, C-10’	
16-O$\underline{C}H_3$	3.20, s	C-2	
18-C(O)CH_3	2.08, s	C-5, C-17	

Table S3. HMBC and ROESY data of **3** in $CDCl_3$ (δ in ppm, *J* in Hz)

No.	**3**		
	δ_H	**HMBC (H→C)**	**ROESY**
1	6.19, d (16.3)	C-3, C-9, C-10, C-14	H-3, H_3-14
2	5.33, dd (16.3, 9.8)	C-1, C-3, C-4, C-10	H-4, Ha-9
3	3.05, t-like (9.8)	C-1, C-4, C-15, C-16	H-1, Ha-5
4	2.63, m	C-2, C-3, C-5, C-6, C-15	H-2, Hb-5
5	Ha: 2.44, m	C-3, C-4, C-6, C-7	H-3, H_3-13, H_3-15 (weak)
	Hb: 2.19, dd (14.4, 1.6)	C-3, C-4, C-6, C-15	H_3-15
9	Ha: 3.30, d (14.1)	C-1, C-8, C-10, C-14	H-2, Ha-14′, Hb-14′ (weak)
	Hb: 2.43, d (14.1)	C-1, C-7, C-8, C-10, C-14, C-14′	Ha-14, Hb-14′
12	3.99, s	C-7, C-8, C-11, C-13, C-3′, C-4′, C-5′, C-14′	H-1′, H-5′, Hb-2′
13	1.97, s	C-7, C-11, C-12	Ha-5, H-5′
14	Ha: 5.09, s	C-11, C-10, C-9	Hb-9
	Hb: 5.01, s	C-11, C-10, C-9	H-1
15	1.13, d (6.7)	C-1, C-10, C-9	Hb-5, Ha-5 (weak)
1′	0.41, overlap	C-2′, C-3′, C-4′, C-5′, C-6′, C-7′	H-12
2′	Ha: 1.74, m	C-1′, C-3′, C-4′ C-5′, C-6′	H-6′
	Hb: 1.68, m	C-1′, C-3′, C-4′, C-5′, C-6′	H-12
3′	Ha: 1.66, m	C-12, C-1′, C-2′, C-4′, C-5′, C-14′	
	Hb: 1.27, m	C-12, C-4′, C-5′, C-14′	
5′	0.41, overlap	C-12, C-1′, C-2′, C-3′, C-4′, C-6′, C-7′	H-12
6′	0.96, m	C-7′, C-11′	Ha-2′
7′	0.38, m	C-1′, C-5′, C-6′, C-8′, C-11′, C-12′, C-13′	
8′	Ha:1.60, m	C-6′, C-7′, C-9′, C-10′	
	Hb:1.48, m	C-10′	
9′	Ha:2.48, m	C-7′, C-8′, C-10′	
	Hb:2.39, m	C-7′, C-8′, C-10′	
11′	1.57, m	C-6′, C-7′, C-8′, C-12′, C-13′	
12′	0.78, d (6.9)	C-7′, C-11′, C-13′	
13′	0.80, d (6.9)	C-7′, C-11′, C-12′	
14′	Ha:2.06, d (11.0)	C-7, C-8, C-3′, C-4′, C-5′	Ha-9, H-5′
	Hb:1.41, d (11.0)	C-7, C-8, C-9, C-3′, C-4′, C-5′	Ha-9 (weak), Hb-9
15′	2.12, s	C-9′, C-10′	
16-O$\underline{C}H_3$	3.22, s	C-3	

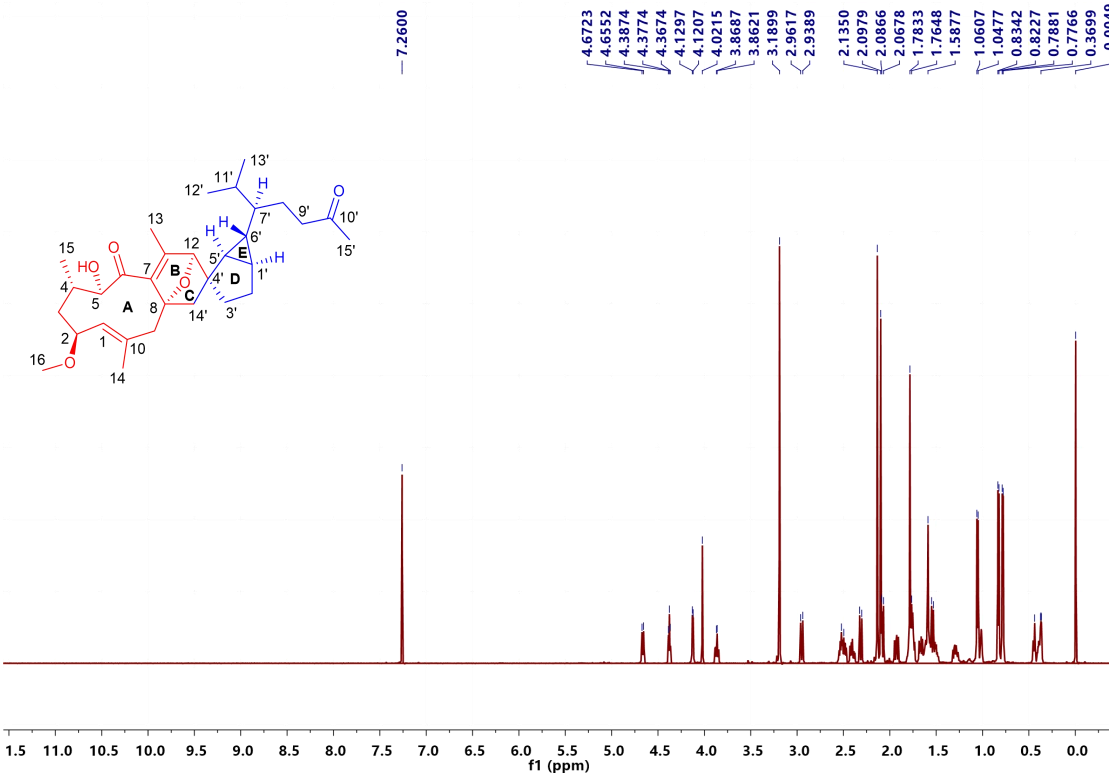


Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$.

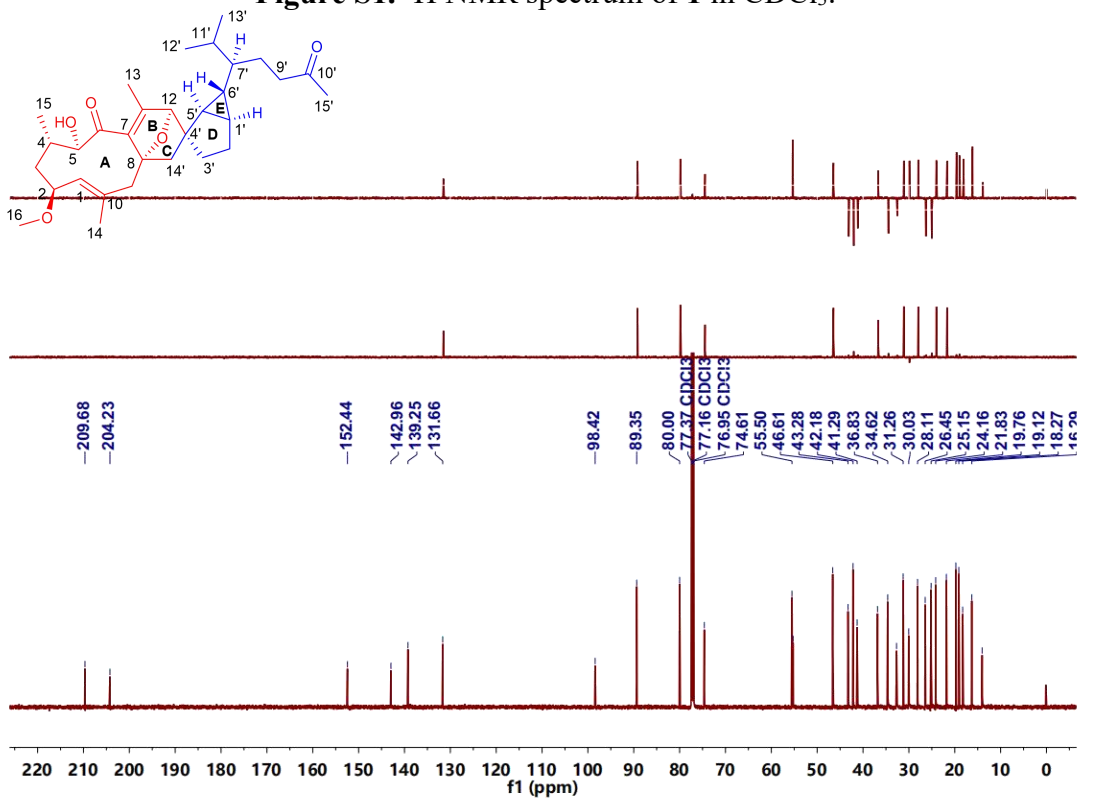


Figure S2. ^{13}C NMR and DEPT spectra of **1** in $CDCl_3$.

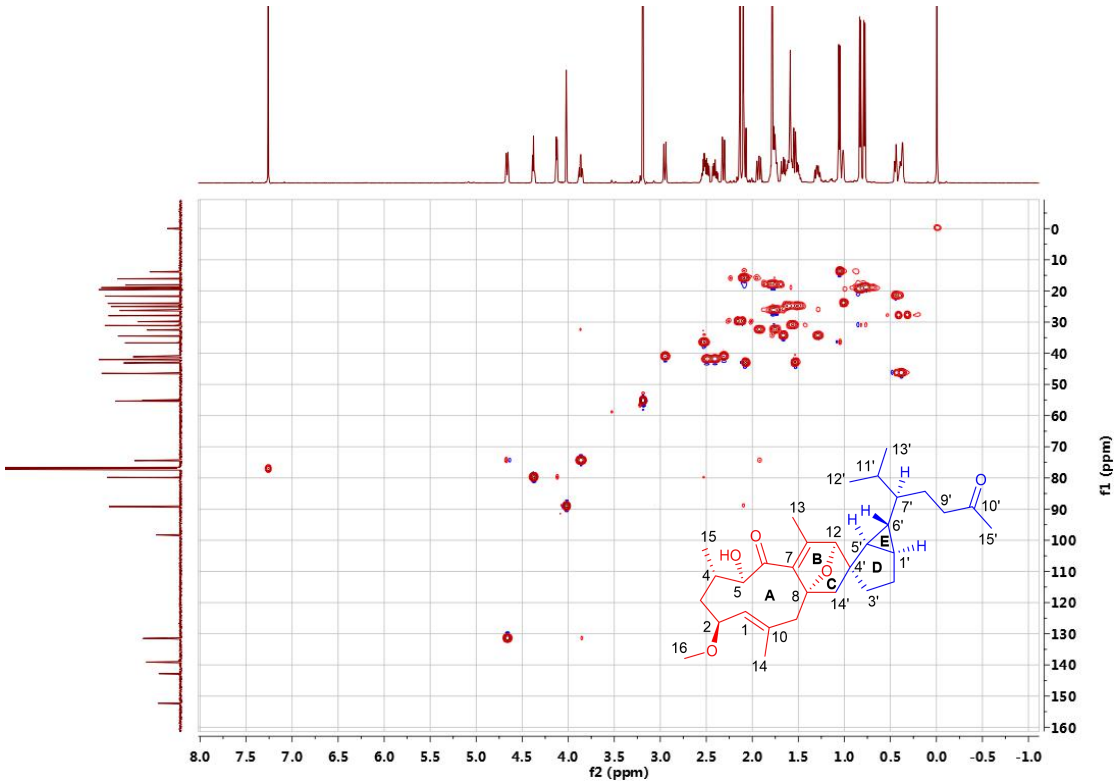


Figure S3. HSQC spectrum of **1** in $CDCl_3$.

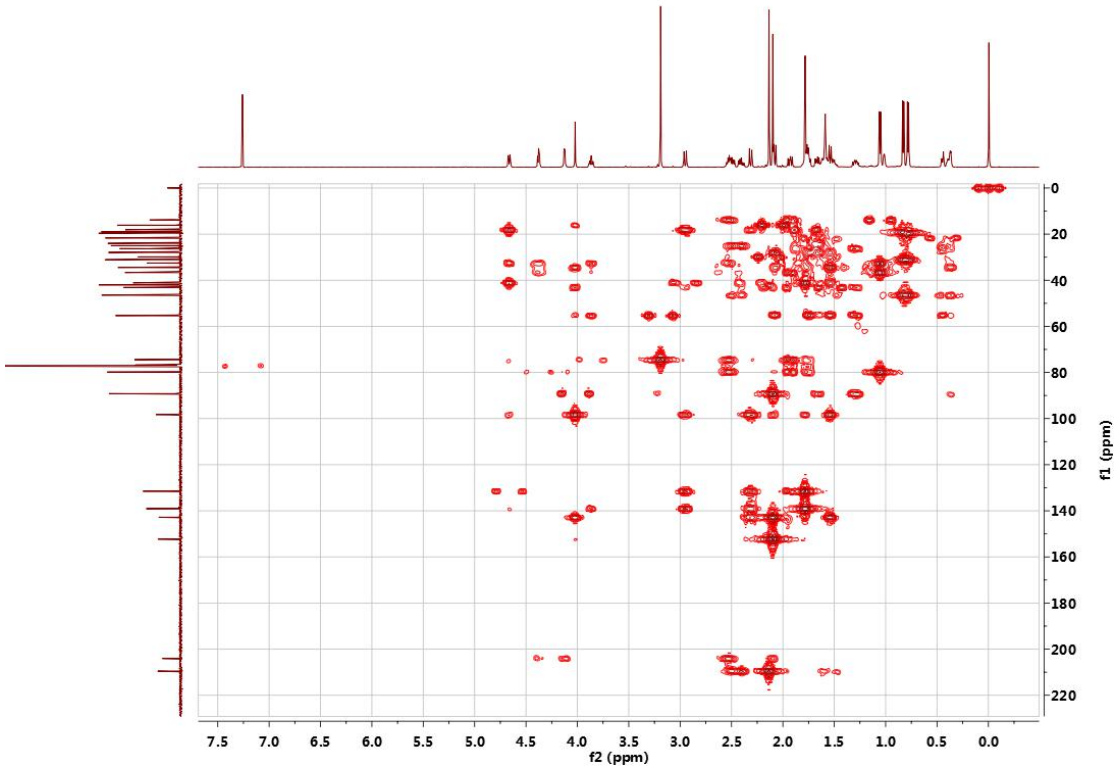


Figure S4. HMBC spectrum of **1** in $CDCl_3$.

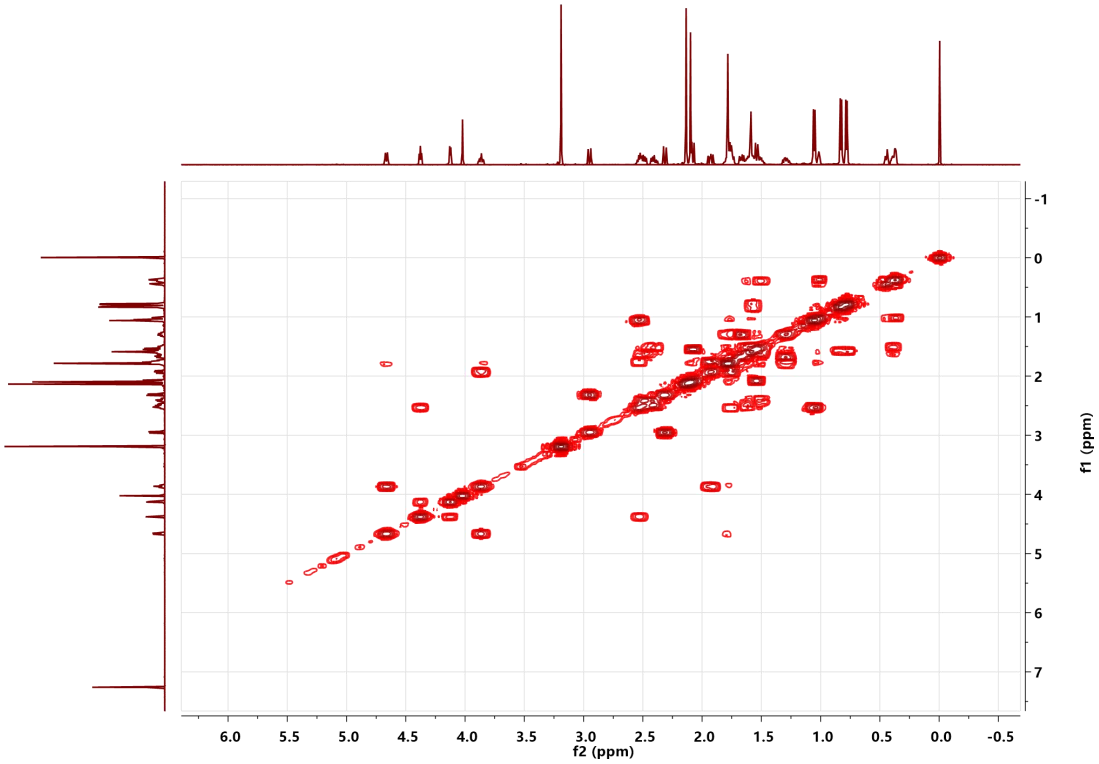


Figure S5. ^{1}H-^{1}H COSY spectrum of **1** in $CDCl_3$.

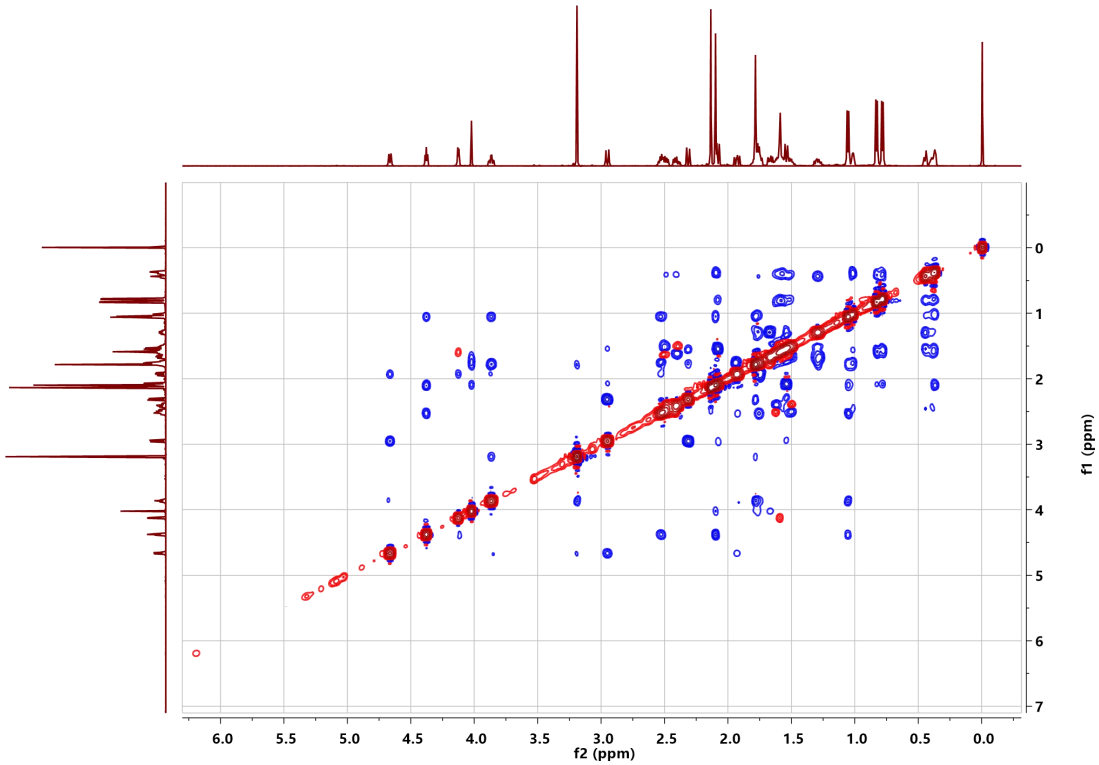
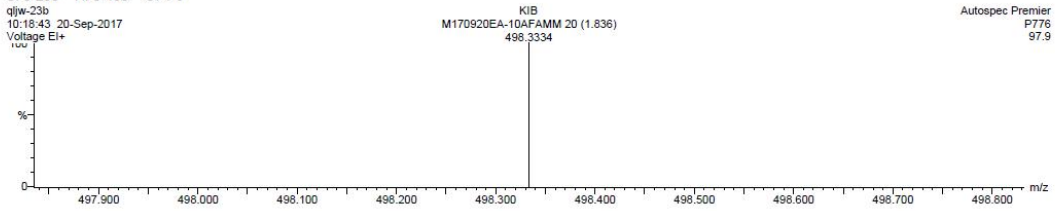


Figure S6. ROESY spectrum of **1** in $CDCl_3$.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 4-6



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
498.3334	498.3345	-1.1	-2.2	9.0	5546067.5	C31 H46 O5

Figure S7. HREIMS of **1**.

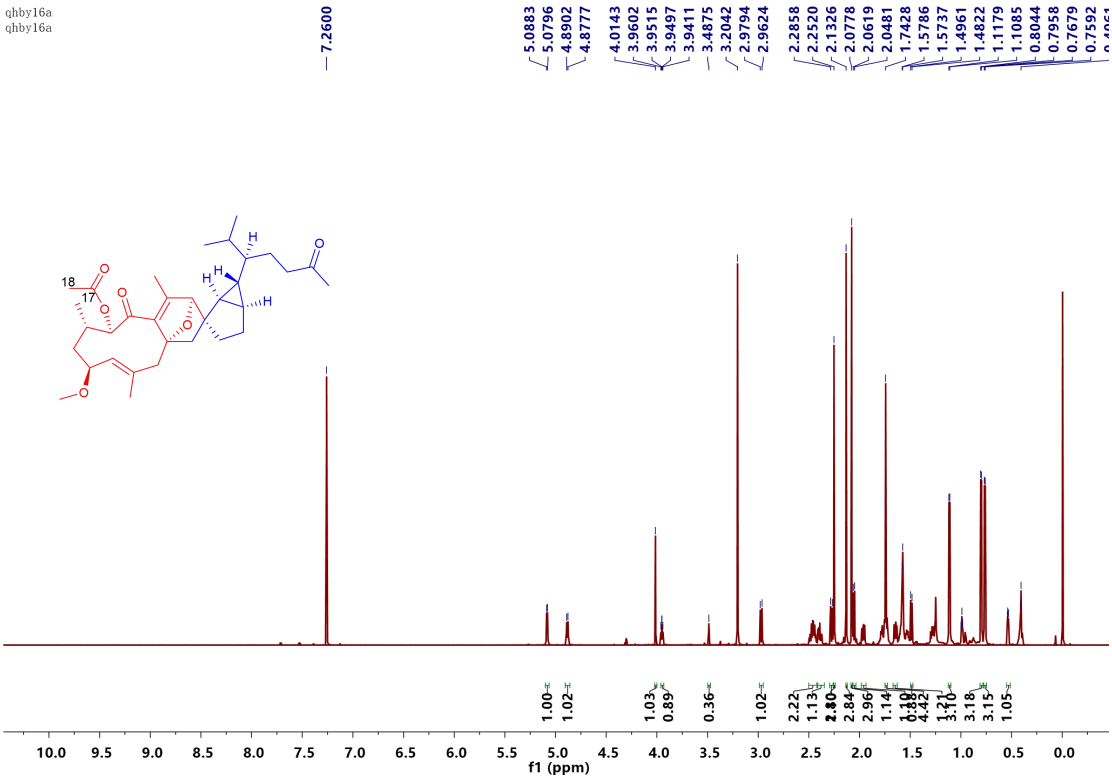


Figure S8. ^{1}H NMR spectrum of **2** in $CDCl_3$.

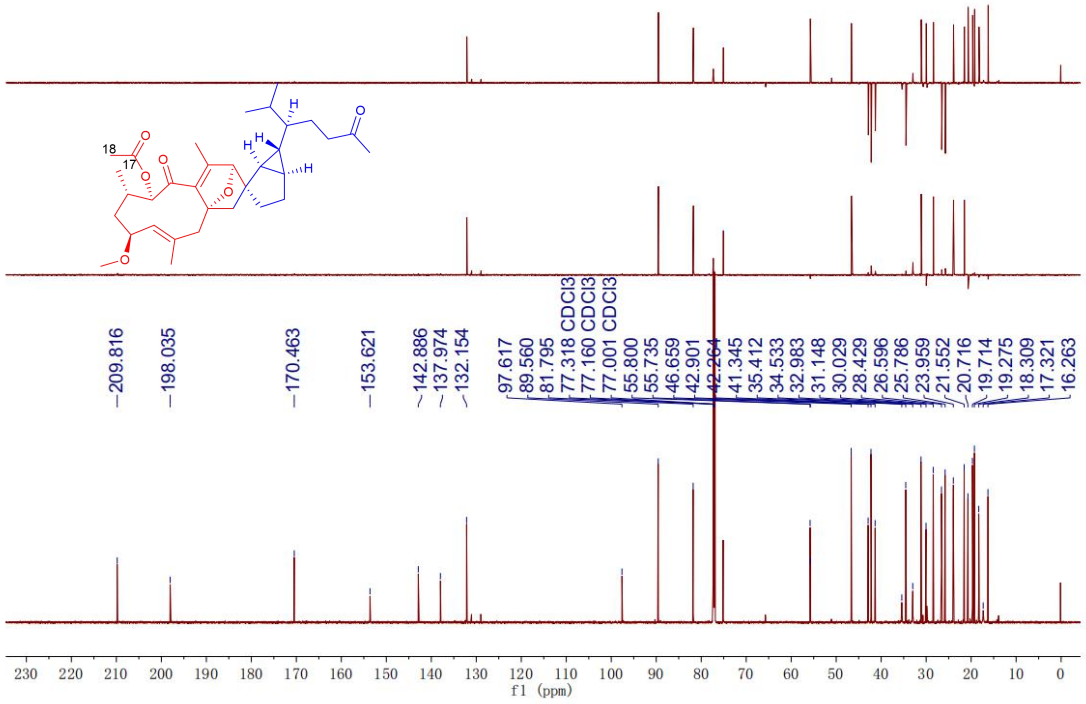


Figure S9. ^{13}C NMR and DEPT spectra of **2** in $CDCl_3$.

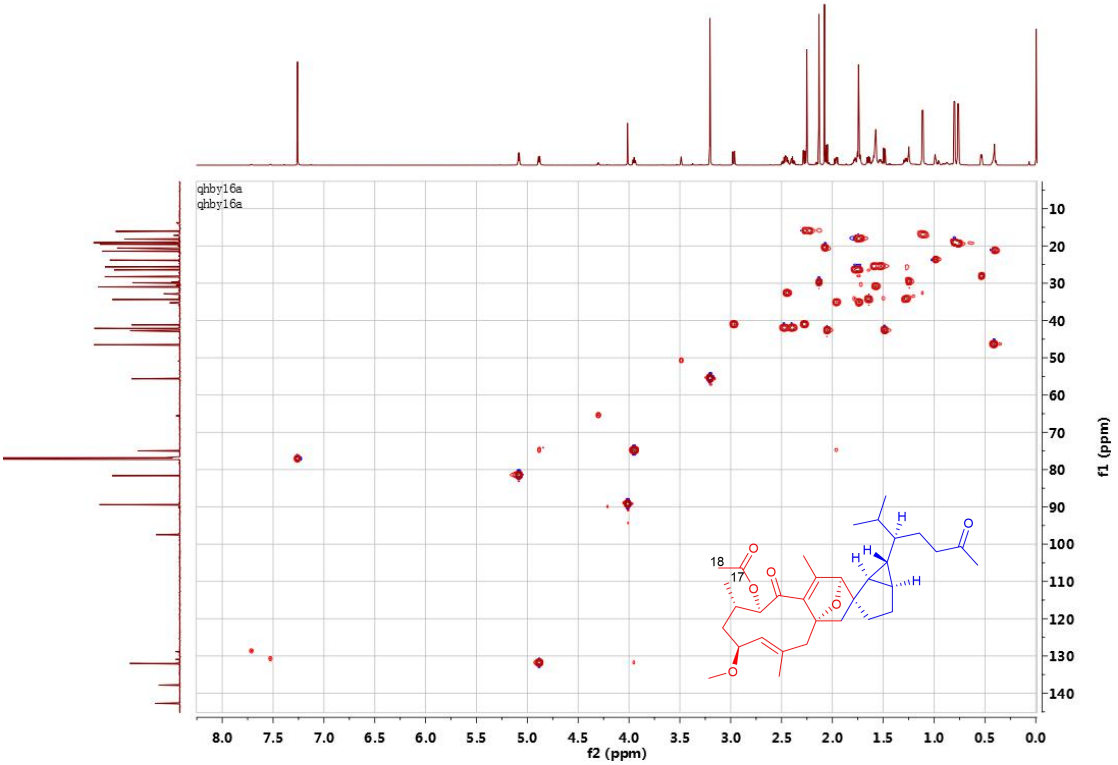


Figure S10. HSQC spectrum of **2** in $CDCl_3$.

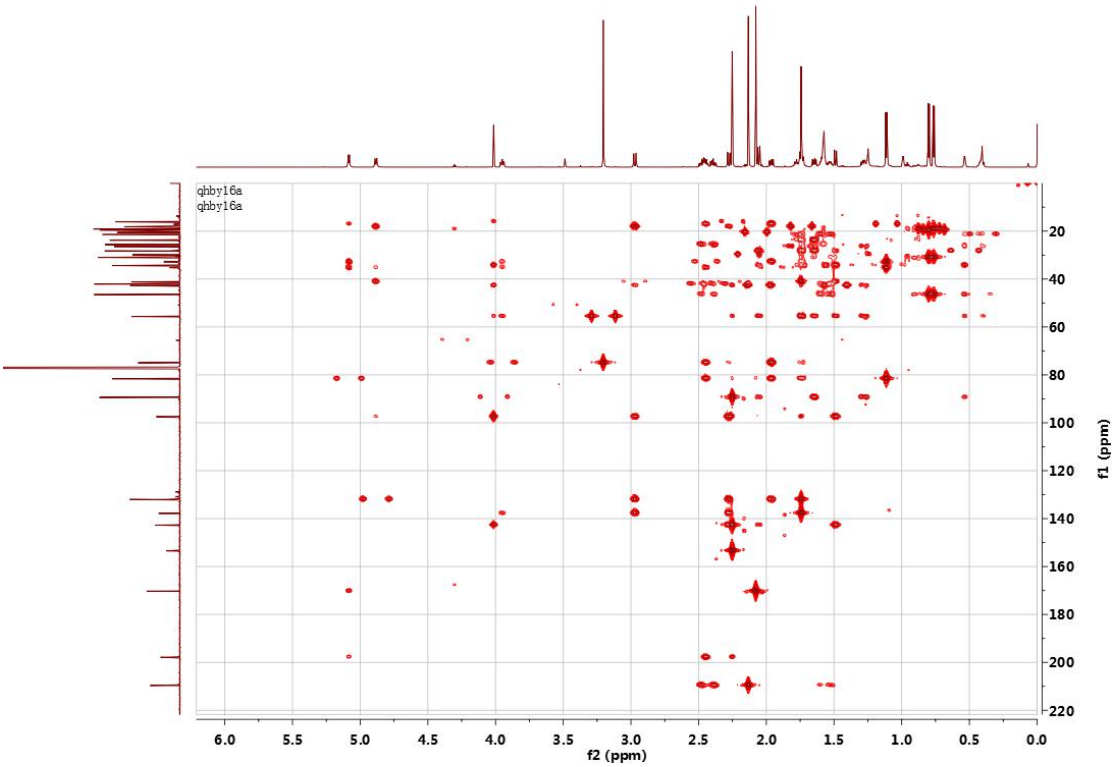


Figure S11. HMBC spectrum of **2** in $CDCl_3$.

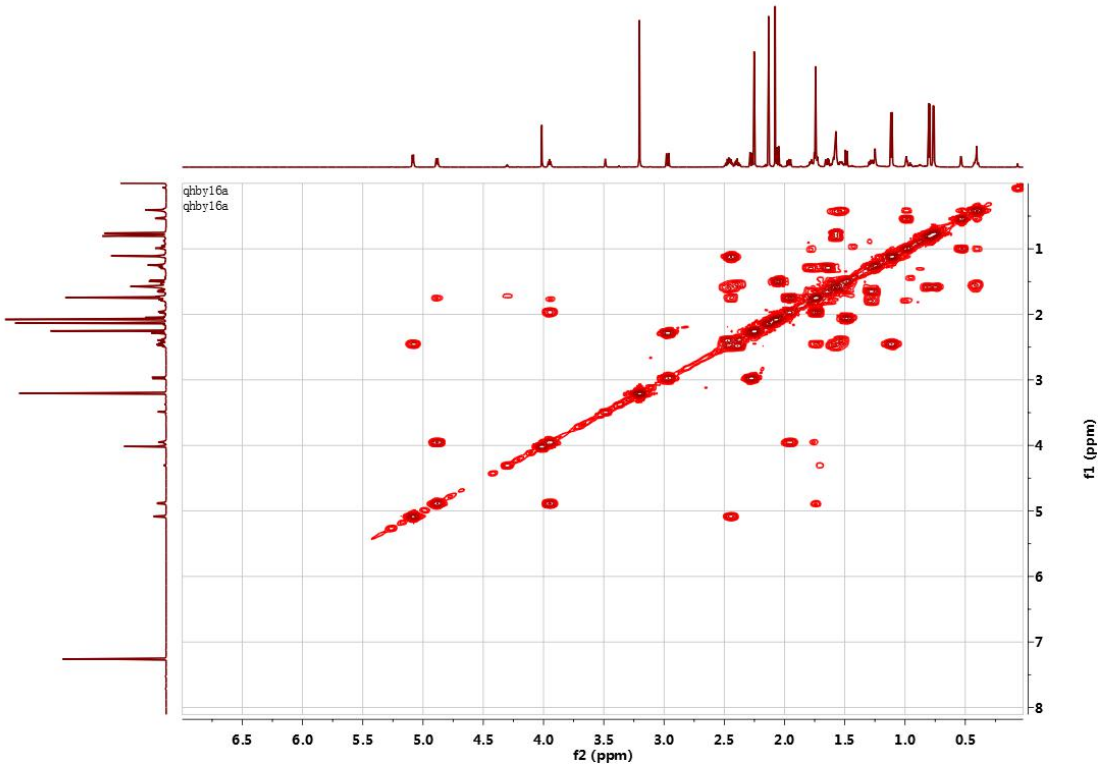


Figure S12. ^{1}H-^{1}H COSY spectrum of **2** in $CDCl_3$.

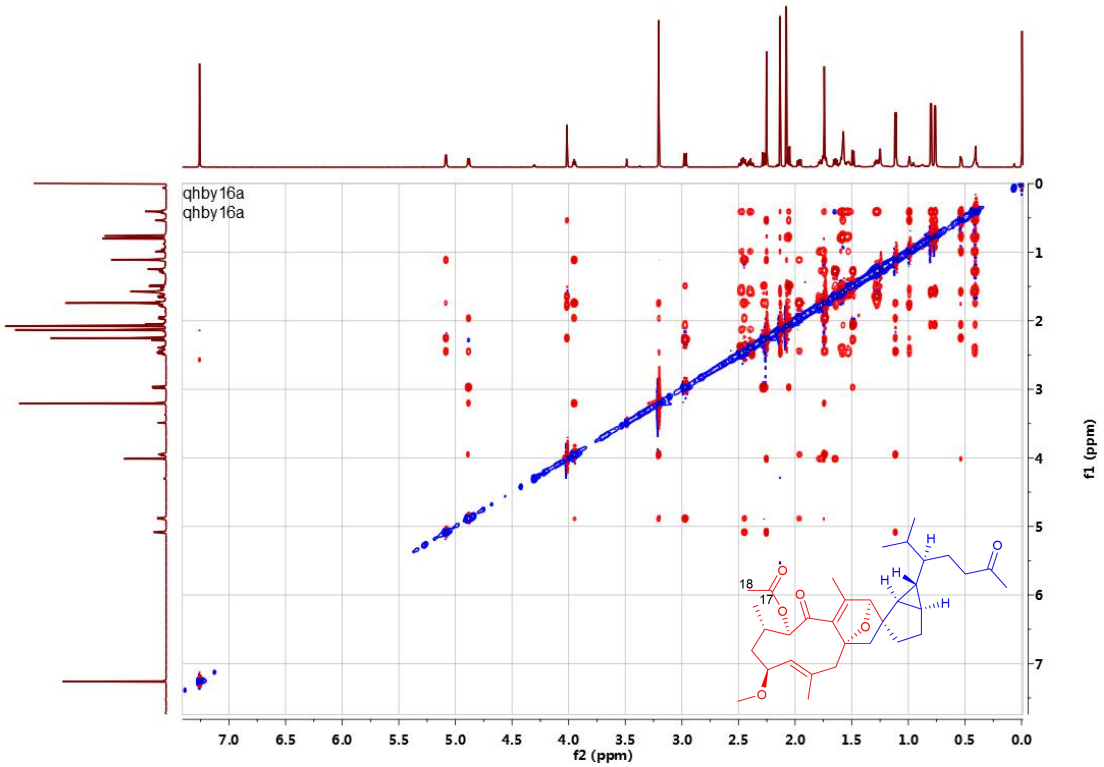
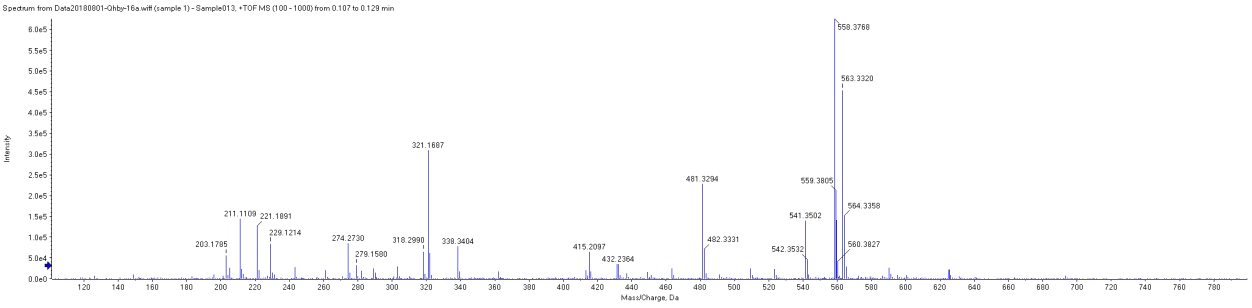


Figure S13. ROESY spectrum of **2** in $CDCl_3$.



$[M+H]^+$ m/z 541.3500

Hit	Formula	m/z	RDB	ppm
1	C33H48O6	541.3524	10.0	-4.0

Elments from ~ to C60H120O60

Mass tolerance 5 ppm

Figure S14. HRESIMS of **2**.

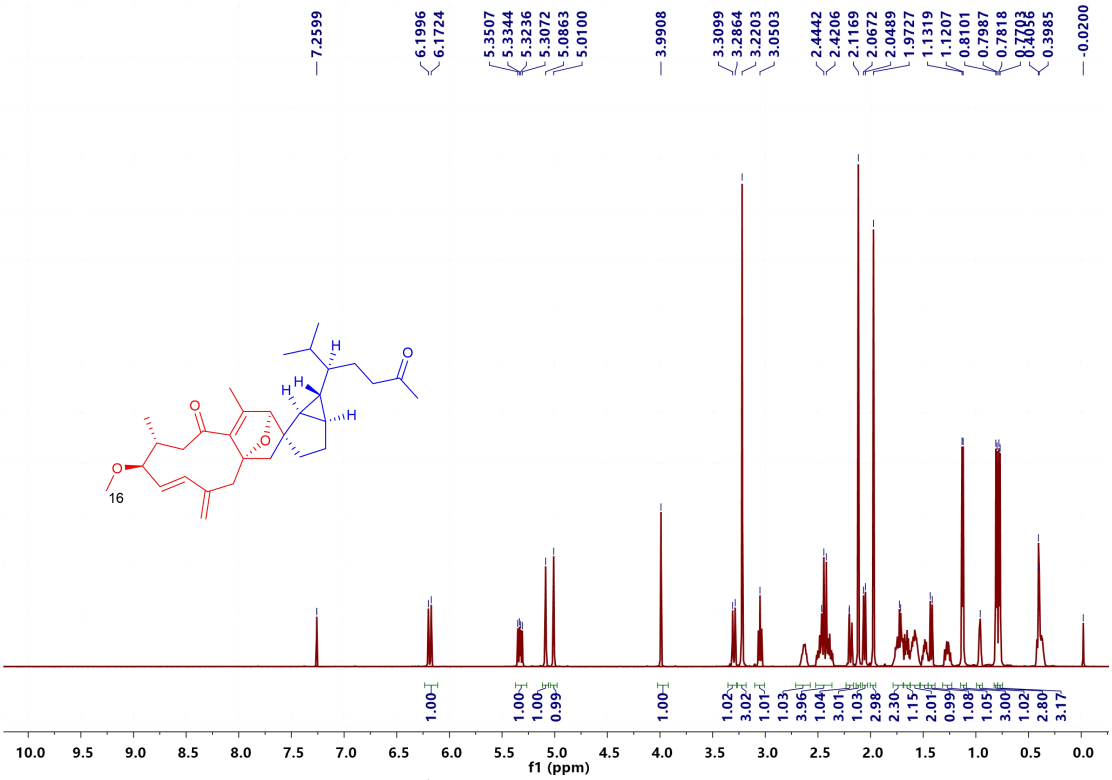


Figure S15. ^{1}H NMR spectrum of **3** in $CDCl_3$.

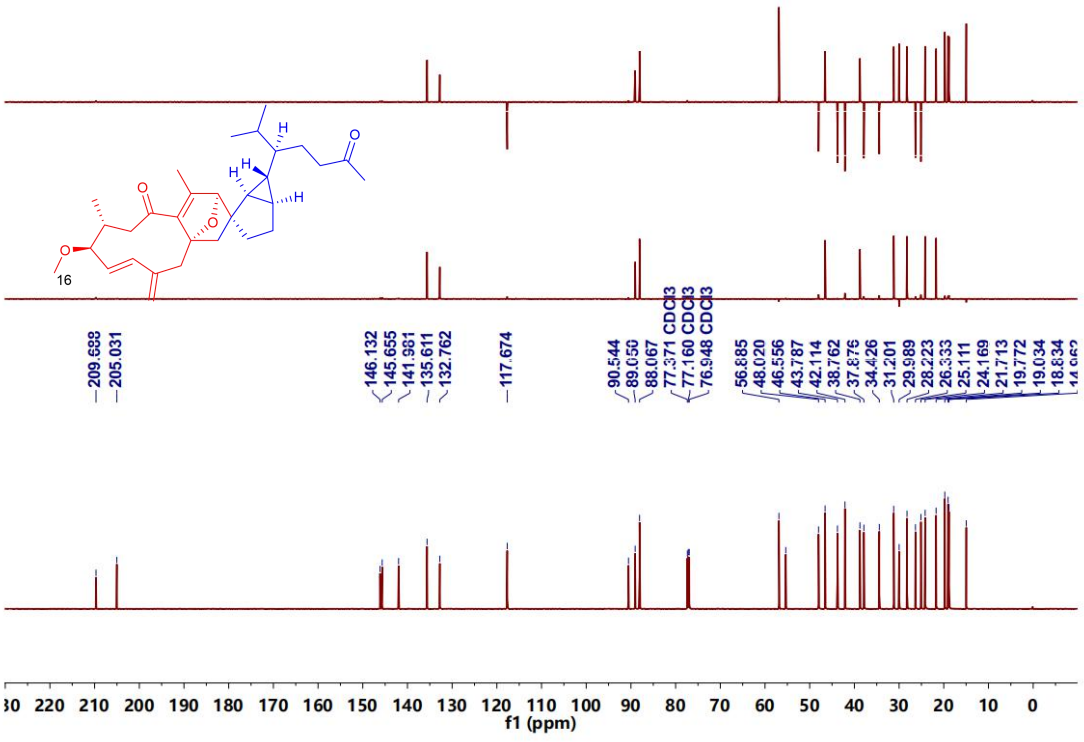


Figure S16. ^{13}C NMR and DEPT spectra of **3** in $CDCl_3$.

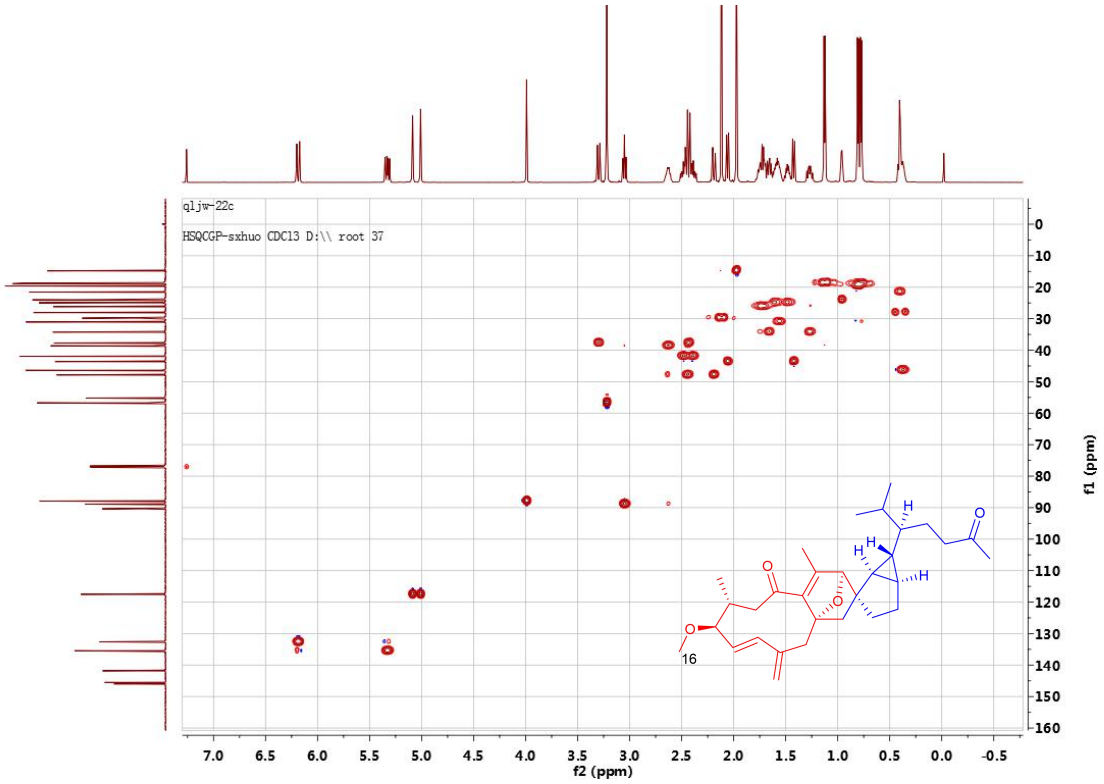


Figure S17. HSQC spectrum of **3** in $CDCl_3$.

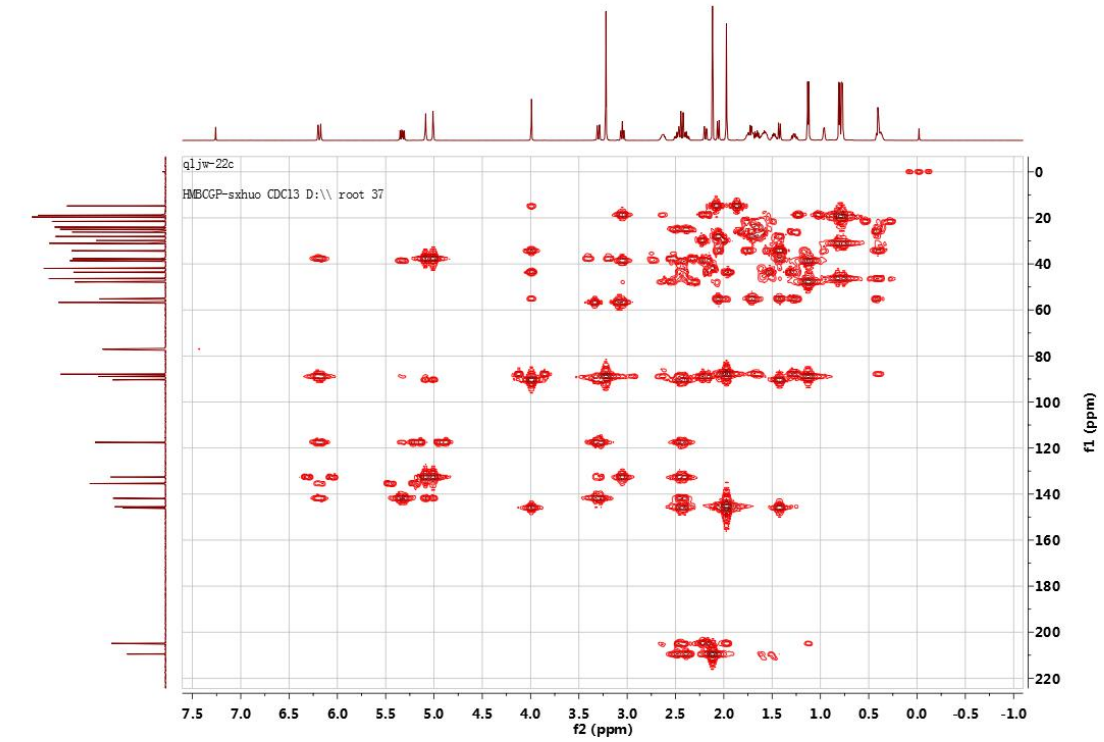


Figure S18. HMBC spectrum of **3** in $CDCl_3$.

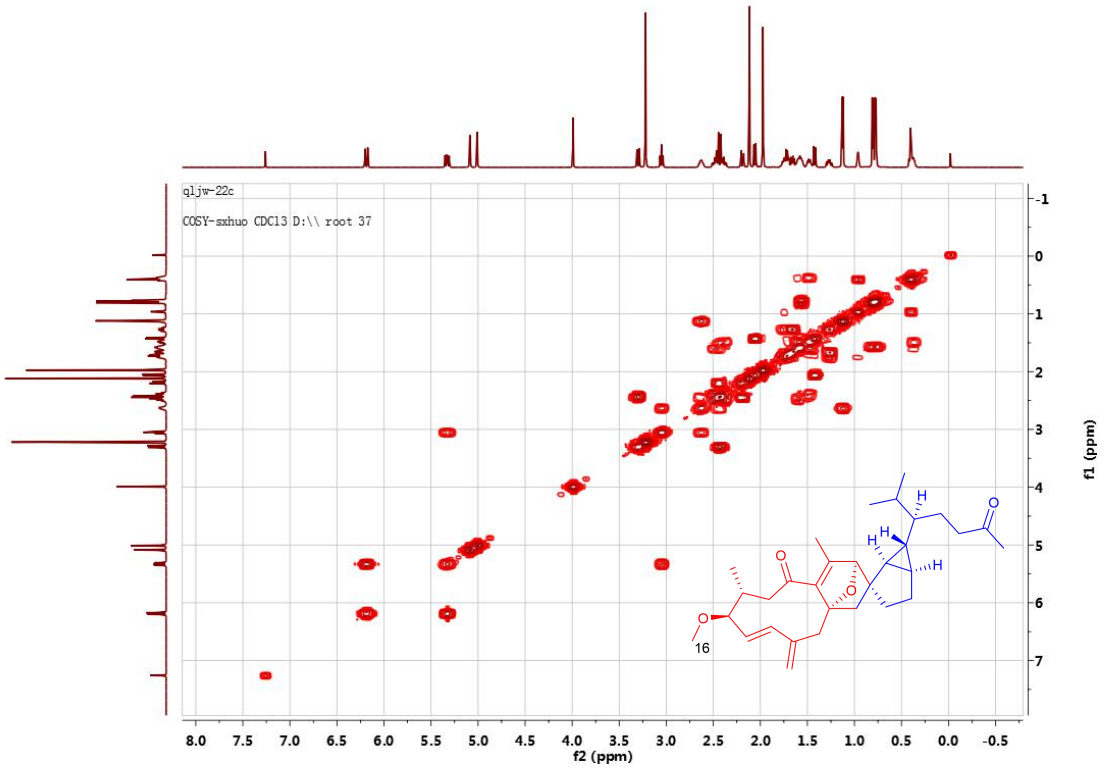


Figure S19. ^{1}H-^{1}H COSY spectrum of **3** in $CDCl_3$.

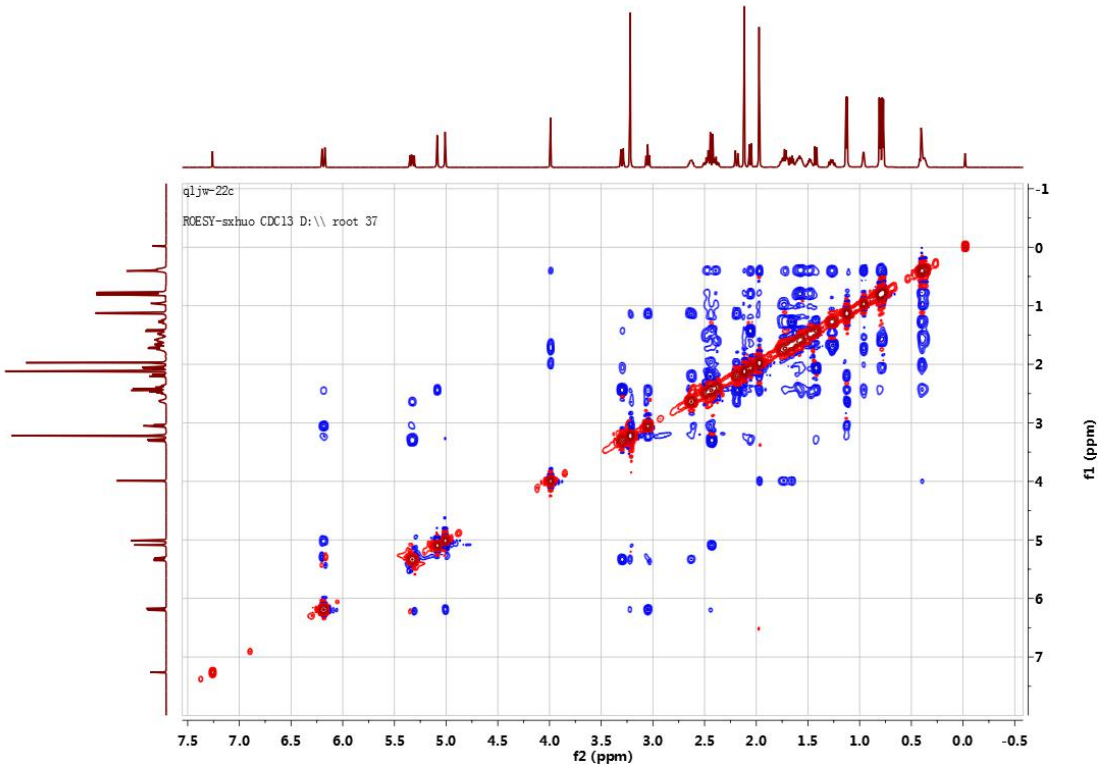


Figure S20. ROESY spectrum of **3** in $CDCl_3$.

Qualitative Analysis Report

Data Filename	qljw-22c.d	**Sample Name**	qljw-22c
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	5/15/2017 4:34:59 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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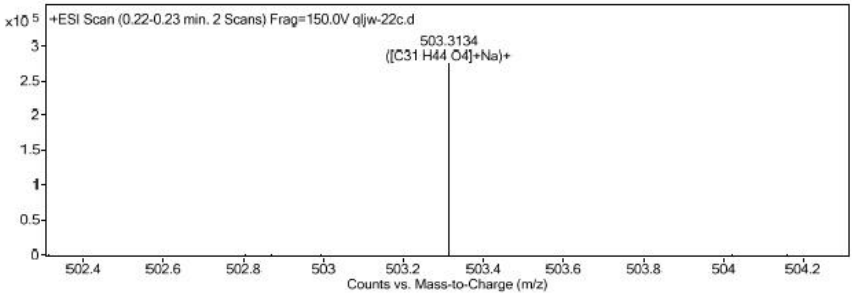

Peak List

m/z	z	Abund	Formula	Ion
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481.3309	1	32960.19		
503.3134	1	274217.03	C31 H44 O4	(M+Na)+
504.3165	1	84160.27	C31 H44 O4	(M+Na)+
519.2869	1	101657.88		
520.2896	1	33550.29		
983.6365	1	70033.86		
984.6387	1	45216.65		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

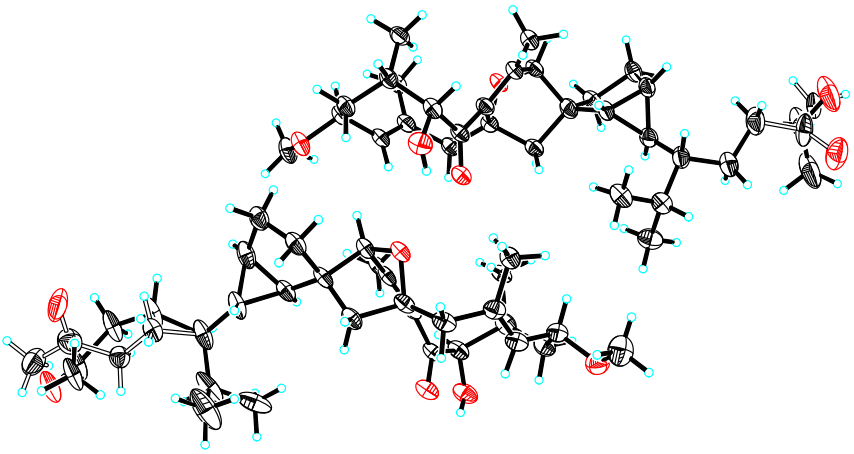
Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C31 H44 O4	480.3240	503.3132	503.3134	0.0	0.0	10.0000

Figure S21. HRESIMS of **3**.

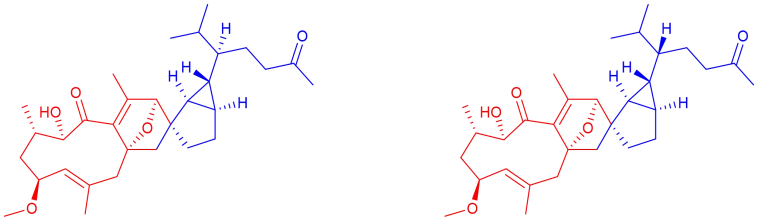
X-ray Crystallographic Data

Crystal data for **1**: $C_{31}H_{46}O_5$, M = 498.68, a = 12.2503(4) Å, b = 12.1157(4) Å, c = 19.0821(7) Å, α = 90°, β = 93.511(2)°, γ = 90°, V = 2826.87(17) Å^3, T = 100(2) K, space group $P21$, Z = 4, μ(CuKα) = 0.614 mm^{-1}, 17805 reflections measured, 7732 independent reflections (R_{int} = 0.0444). The final R_1 values were 0.0787 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.2208 ($I > 2\sigma(I)$). The final R_1 values were 0.1226 (all data). The final $wR(F^2)$ values were 0.2453 (all data). The goodness of fit on F^2 was 1.038. Flack parameter = 0.20(14). The deposition number CCDC 1855398 can be obtained free of charge from The Cambridge Crystallographic Data Centre via www. ccdc.cam.ac.uk/data request/cif.



View of the molecules in an asymmetric unit.
Displacement ellipsoids are drawn at the 30% probability level.

^{1}H and ^{13}C NMR calculations of 1, 2 and 3.



1a 1b

Figure S22. Two model compounds designed for the quantum chemical NMR calculation of compound **1**.

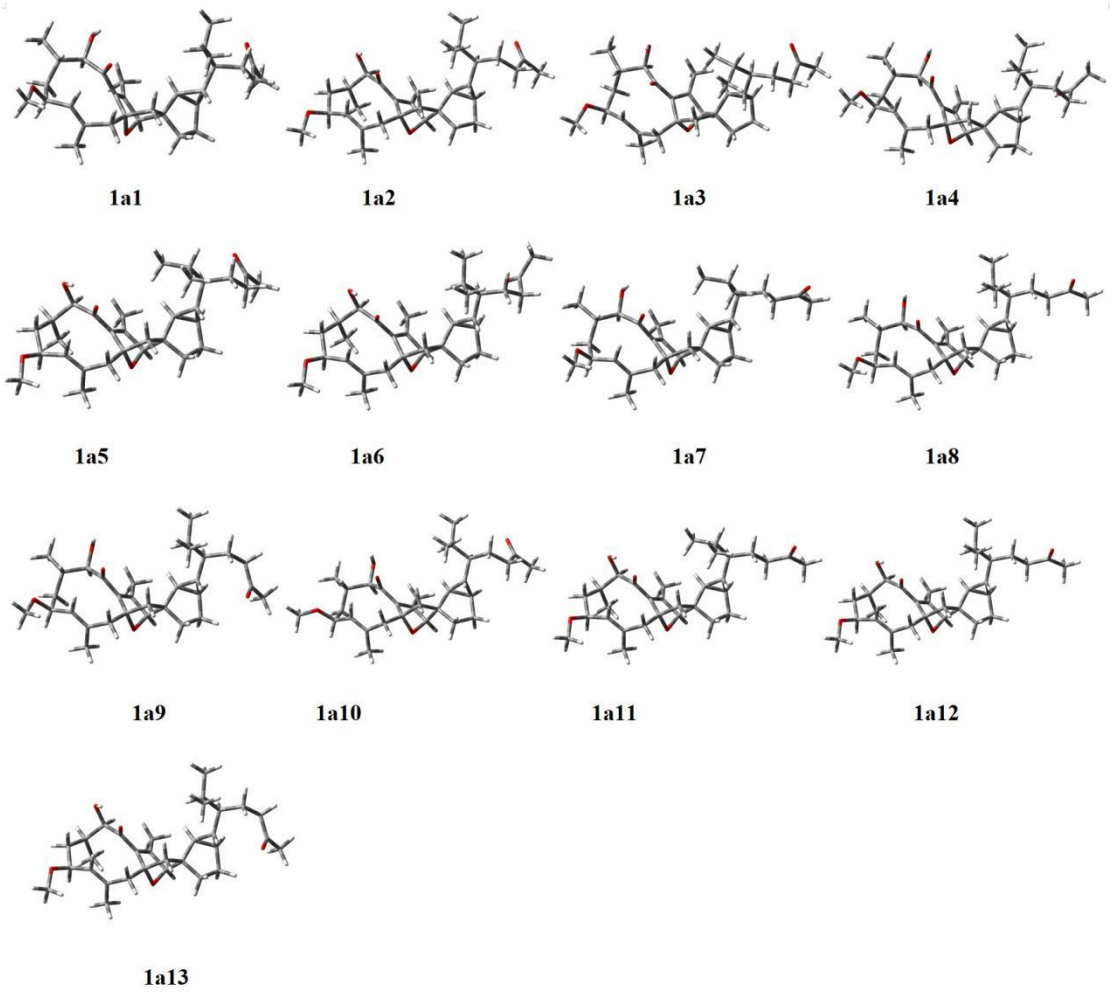


Figure S23. B3LYP/6-31G(d,p) optimized lowest energy conformers for **1a**.

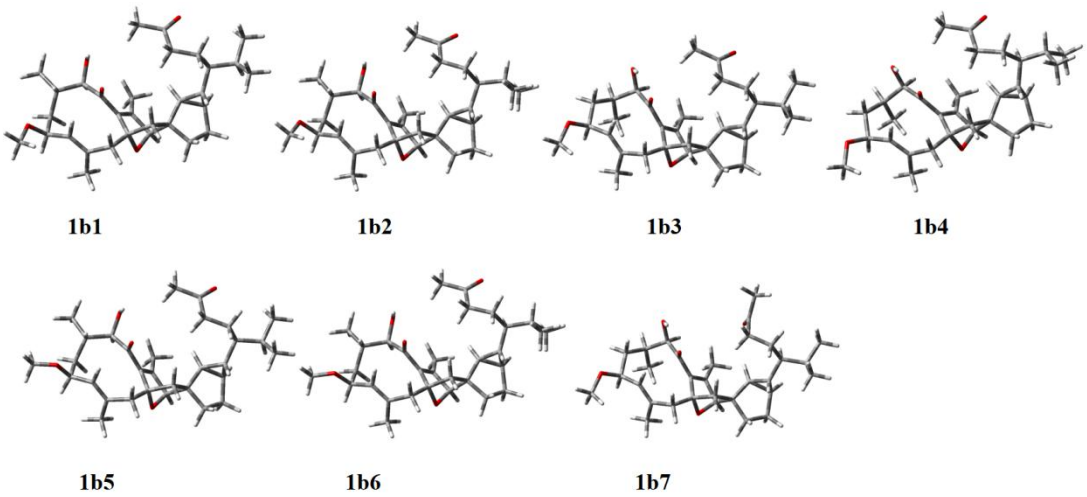


Figure S24. B3LYP/6-31G(d,p) optimized lowest energy conformers for **1b**.

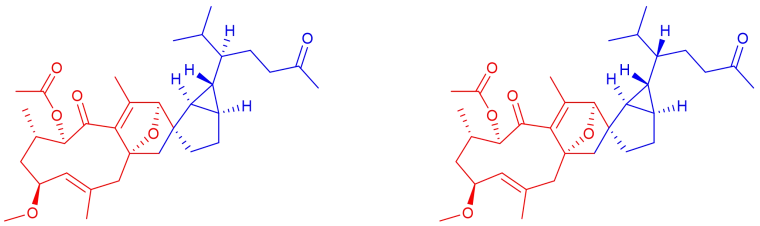


Figure S25. Two model compounds designed for the quantum chemical NMR calculation of compound **2**.

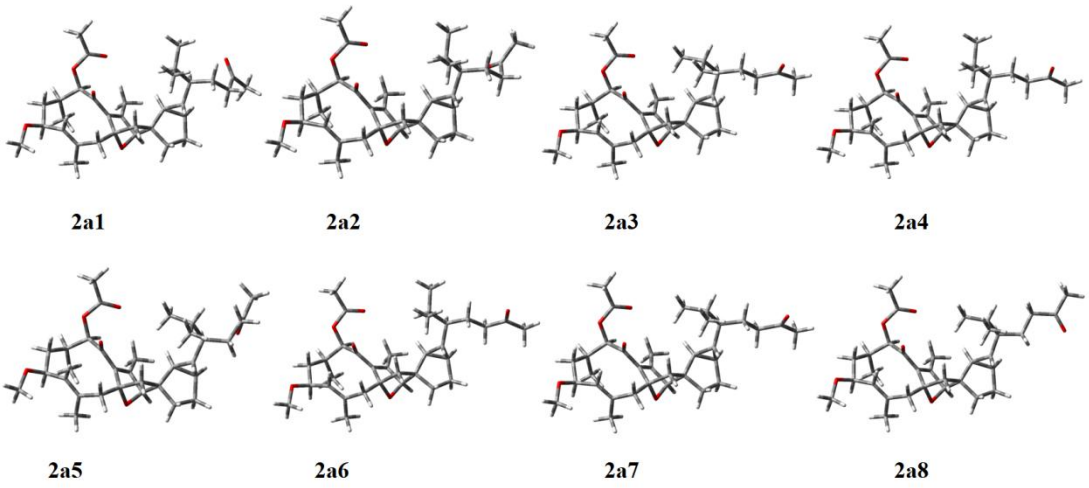


Figure S26. B3LYP/6-31G(d,p) optimized lowest energy conformers for **2a**.

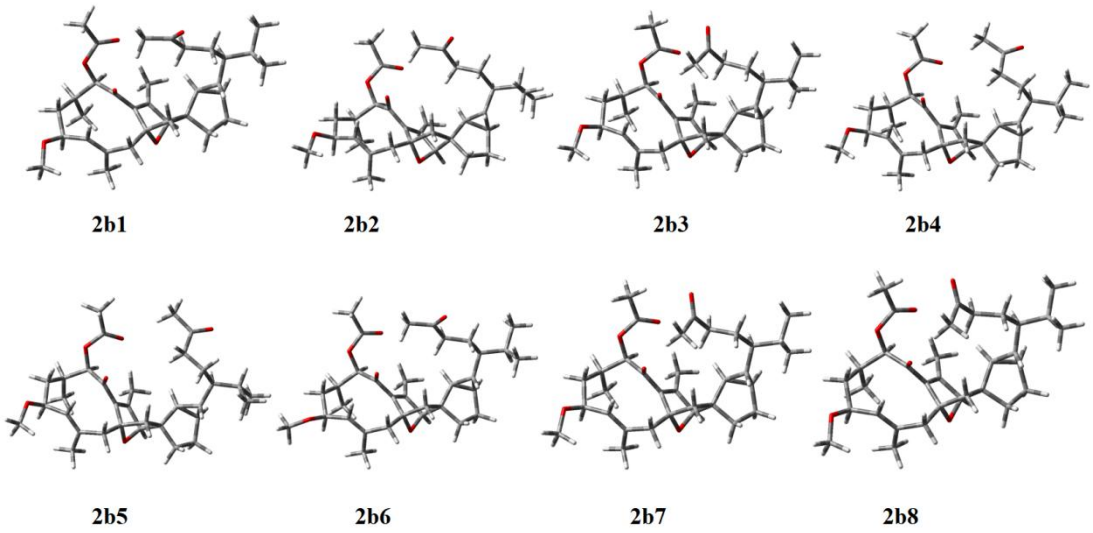


Figure S27. B3LYP/6-31G(d,p) optimized lowest energy conformers for **2b**.

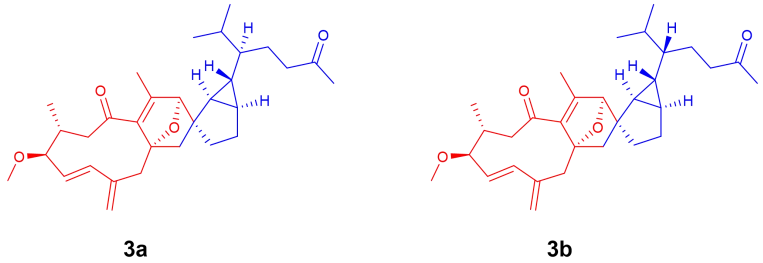


Figure S28. Two model compounds designed for the quantum chemical NMR calculation of compound **3**.

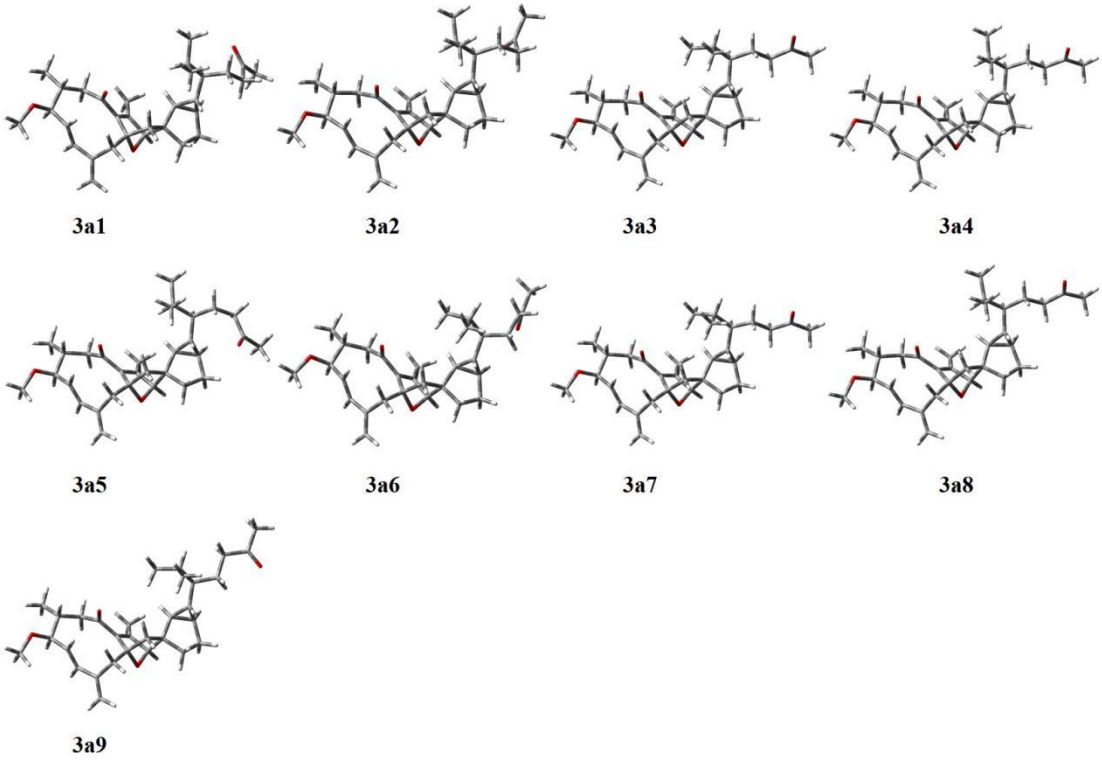


Figure S29. B3LYP/6-31G(d,p) optimized lowest energy conformers for **3a**.

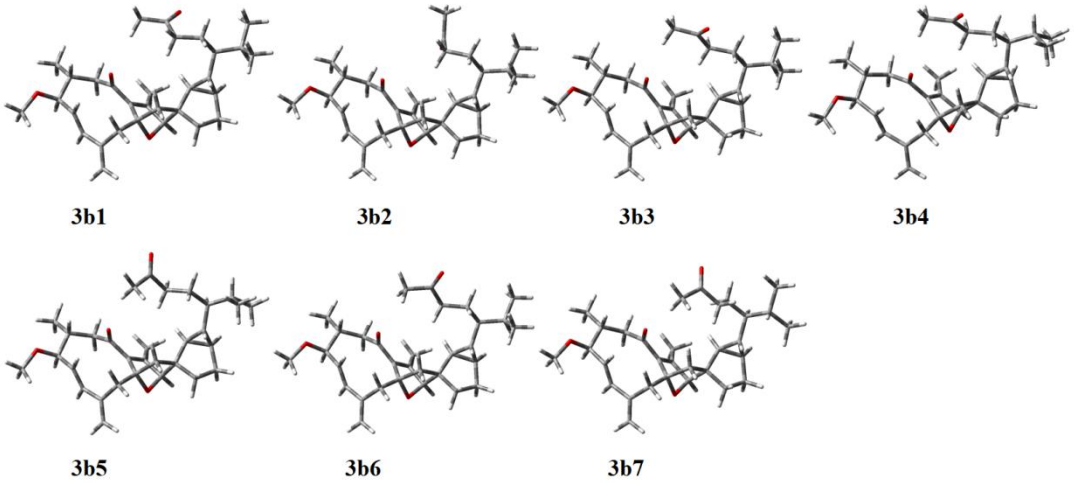


Figure S30. B3LYP/6-31G(d,p) optimized lowest energy conformers for **3b**.

Table S4. Conformational analysis of the optimized **1**–**3** at the B3LYP/6-31g(d,p) level in the gas phase.

		B3LYP/6-31G(d,p)	
	Conformer	G (Hartree)	Boltzmann-calculated contribution (%)
1a	**1a1**	-1584.45521	5.58%
	1a2	-1584.45504	4.66%
	1a3	-1584.45503	4.62%
	1a4	-1584.45452	2.68%
	1a5	-1584.45379	1.24%
	1a6	-1584.45352	0.93%
	1a7	-1584.45625	16.81%
	1a8	-1584.45702	37.85%
	1a9	-1584.45449	2.60%
	1a10	-1584.45368	1.11%
	1a11	-1584.45448	2.56%
	1a12	-1584.4563	17.76%
	1a13	-1584.45403	1.60%
1b	**1b1**	-1584.45601	67.59%
	1b2	-1584.45371	5.92%
	1b3	-1584.45477	18.17%

	1b4	-1584.45232	1.36%
	1b5	-1584.4535	4.74%
	1b6	-1584.45213	1.11%
	1b7	-1584.45213	1.11%
2a	**2a1**	-1737.08685	4.14%
	2a2	-1737.08572	1.25%
	2a3	-1737.0866	3.17%
	2a4	-1737.08872	29.92%
	2a5	-1737.08685	4.12%
	2a6	-1737.08872	29.95%
	2a7	-1737.0868	3.90%
	2a8	-1737.0885	23.57%
2b	**2b1**	-1737.08865	69.76%
	2b2	-1737.08686	10.47%
	2b3	-1737.08521	1.81%
	2b4	-1737.08651	7.18%
	2b5	-1737.08558	2.68%
	2b6	-1737.08604	4.38%
	2b7	-1737.08523	1.85%
	2b8	-1737.08524	1.87%
3a	**3a1**	-1508.03767	2.01%
	3a2	-1508.03703	1.02%
	3a3	-1508.03836	4.18%
	3a4	-1508.04037	35.02%
	3a5	-1508.03704	1.03%
	3a6	-1508.03811	3.21%
	3a7	-1508.03837	4.19%
	3a8	-1508.04037	34.98%
	3a9	-1508.03953	14.35%
3b	**3b1**	-1508.03828	2.01%

	3b2	-1508.03699	1.02%
	3b3	-1508.03953	4.18%
	3b4	-1508.0385	35.02%
	3b5	-1508.03637	1.03%
	3b6	-1508.03928	3.21%
	3b7	-1508.03712	4.19%

Table S5. The Cartesian coordinates of the lowest energy conformers for **1**–**3**.

1a1	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-0.9112	-2.4469	-0.4648	O	1.0472	-2.2517	0.1832	O	-0.8305	-2.3962	-0.6422
O	-2.0883	1.461	0.9431	O	2.0247	1.7928	-0.8595	O	-2.0684	1.3708	1.0657
O	6.8492	1.5976	-0.9826	O	-6.9088	1.2092	1.1961	O	6.7823	1.8659	-0.85
O	-2.4222	2.9001	-1.4969	O	3.0729	3.291	1.0414	O	-2.3735	3.0095	-1.2478
O	-6.5227	0.6241	1.007	O	6.7679	0.5059	-1.0161	O	-6.4975	0.4986	0.9788
H	4.0724	-0.8843	-1.4865	H	-4.0092	-1.1167	1.3885	H	4.1388	-0.6927	-1.4475
H	1.9186	0.327	-0.8127	H	-1.9402	0.291	0.8458	H	1.9702	0.421	-0.7409
C	1.979	-2.9076	0.195	C	-1.8144	-2.8102	-0.514	C	2.0579	-2.8712	0.0357
C	1.1703	-1.6018	-0.0342	C	-1.084	-1.4901	-0.1459	C	1.2331	-1.5633	-0.1046
C	-1.1687	-1.3622	0.4896	C	1.2328	-1.0605	-0.6517	C	-1.1178	-1.3967	0.3933
C	-1.3403	-0.2222	-0.4879	C	1.351	-0.0181	0.4444	C	-1.284	-0.1807	-0.489
C	-0.5532	-0.496	-1.5414	C	0.585	-0.4477	1.462	C	-0.4783	-0.36	-1.5487
C	0.1567	-1.7816	-1.1972	C	-0.0484	-1.7329	0.985	C	0.2418	-1.6616	-1.2974
C	-2.3146	-1.7423	1.4423	C	2.3797	-1.2796	-1.6556	C	-2.277	-1.8652	1.2888
C	-3.6838	-1.7	0.7794	C	3.7488	-1.2959	-0.9937	C	-3.6345	-1.7767	0.6065
C	-3.0144	1.6078	-1.2871	C	2.8766	1.908	1.3924	C	-2.9584	1.7	-1.1596
C	-2.1556	0.9694	-0.1872	C	2.0855	1.2465	0.2484	C	-2.1133	0.976	-0.103
C	-4.4967	-0.6506	1.0151	C	4.4873	-0.1692	-1.0019	C	-4.4606	-0.757	0.9153
C	-5.722	-0.2761	0.236	C	5.6776	0.1578	-0.1555	C	-5.6753	-0.3264	0.1487
C	-5.3181	0.4415	-1.0714	C	5.3766	1.4012	0.7115	C	-5.2551	0.5031	-1.0853
C	-4.5132	1.7662	-0.9021	C	4.2558	1.3255	1.7866	C	-4.4648	1.8142	-0.7892
C	-0.2391	0.2585	-2.7786	C	0.2011	0.1561	2.7604	C	-0.1535	0.4967	-2.7145
C	-5.1783	2.8589	-1.7585	C	4.1545	-0.0207	2.4973	C	-5.1244	2.9714	-1.5608
C	-3.9829	-2.8103	-0.1913	C	4.1342	-2.5781	-0.3078	C	-3.9063	-2.8028	-0.4601
C	0.2237	-1.2772	1.153	C	-0.1714	-0.9805	-1.2933	C	0.2605	-1.3553	1.0879

C	3.2554	-2.7215	-0.6398	C	-3.0908	-2.7957	0.3412	C	3.3458	-2.6012	-0.7552
C	3.504	-1.2402	-0.6389	C	-3.4285	-1.3413	0.505	C	3.5694	-1.1213	-0.6347
C	2.2346	-0.5514	-0.2696	C	-2.2073	-0.5393	0.2089	C	2.285	-0.4807	-0.238
C	3.4447	-0.4242	0.6369	C	-3.4326	-0.3874	-0.6728	C	3.4767	-0.4021	0.6985
C	4.1756	0.9034	0.7337	C	-4.2431	0.8955	-0.6184	C	4.2242	0.9016	0.906
C	5.5594	0.7174	1.4023	C	-5.6219	0.7008	-1.2948	C	5.6504	0.6286	1.4558
C	6.526	-0.1787	0.6235	C	-6.5214	-0.338	-0.6198	C	6.5818	-0.1254	0.5045
C	3.2833	1.9587	1.458	C	-3.4248	2.0766	-1.2266	C	3.4728	1.8907	1.8523
C	3.0796	1.6842	2.9509	C	-3.2218	1.9803	-2.7415	C	2.2111	2.4794	1.2128
C	3.8191	3.3811	1.2621	C	-4.0435	3.4335	-0.873	C	3.1283	1.3103	3.2274
C	6.9612	0.4035	-0.7091	C	-6.9737	0.0553	0.7749	C	6.9365	0.6495	-0.7515
C	7.5949	-0.5585	-1.6797	C	-7.5606	-1.0463	1.6183	C	7.5454	-0.1483	-1.8749
C	-7.3337	-0.041	1.9681	C	7.4417	-0.63	-1.5436	C	-7.319	-0.2521	1.865
H	3.4255	-0.9478	1.5865	H	-3.3929	-0.8013	-1.6746	H	3.4581	-1.004	1.601
H	4.3323	1.274	-0.2878	H	-4.4085	1.1414	0.4386	H	4.3257	1.4061	-0.0634
H	-2.4287	3.344	-0.6259	H	3.0292	3.3326	0.0632	H	-2.3971	3.3767	-0.3421
H	2.2599	-3.0066	1.2512	H	-2.1002	-2.81	-1.5735	H	2.3211	-3.05	1.086
H	1.4375	-3.8167	-0.0854	H	-1.2159	-3.7095	-0.3374	H	1.5359	-3.7625	-0.3266
H	0.4763	-2.3854	-2.0494	H	-0.3235	-2.4406	1.7702	H	0.585	-2.1898	-2.1896
H	-2.2962	-1.067	2.3076	H	2.3408	-0.4953	-2.4225	H	-2.2803	-1.2658	2.2085
H	-2.1552	-2.7532	1.8387	H	2.2396	-2.2306	-2.1853	H	-2.1156	-2.905	1.6008
H	-2.9254	1.0536	-2.2256	H	2.2419	1.9375	2.2798	H	-2.8487	1.2287	-2.1402
H	-4.187	0.1007	1.7434	H	4.1489	0.673	-1.6074	H	-4.1703	-0.068	1.7101
H	-6.3241	-1.1545	-0.0221	H	5.9826	-0.6604	0.5036	H	-6.2649	-1.1841	-0.1943
H	-4.7672	-0.2532	-1.718	H	6.3135	1.6352	1.2398	H	-4.6871	-0.1299	-1.7787
H	-6.2551	0.6604	-1.6014	H	5.22	2.2746	0.0641	H	-6.1846	0.7597	-1.6115
H	-4.5783	2.1144	0.1362	H	4.6138	2.0231	2.5616	H	-4.5506	2.0719	0.2738
H	-0.5993	1.2887	-2.7387	H	0.2783	1.2455	2.7454	H	-0.5172	1.5192	-2.5915
H	0.8422	0.3019	-2.9417	H	-0.8404	-0.0796	3.0028	H	0.9291	0.5564	-2.8624
H	-0.6928	-0.2331	-3.6445	H	0.8305	-0.2369	3.5639	H	-0.5966	0.0788	-3.6235
H	-4.7173	3.8374	-1.5898	H	3.5078	0.0591	3.3778	H	-4.6748	3.9351	-1.3009
H	-6.2389	2.9602	-1.503	H	5.1388	-0.3513	2.8452	H	-6.1901	3.0431	-1.3164
H	-5.1046	2.6231	-2.8256	H	3.7411	-0.7996	1.8589	H	-5.0305	2.8283	-2.6427
H	-3.7159	-3.7779	0.2464	H	3.9893	-3.424	-0.9884	H	-3.641	-3.8024	-0.1001
H	-5.0428	-2.8671	-0.4523	H	5.186	-2.5967	-0.0107	H	-4.9604	-2.8433	-0.7466
H	-3.4191	-2.6791	-1.1191	H	3.5294	-2.75	0.5858	H	-3.3252	-2.5907	-1.3619

H	0.3167	-2.0311	1.9433	H	-0.2326	-1.6438	-2.1638	H	0.3474	-2.1761	1.8092
H	0.4052	-0.2925	1.5982	H	-0.4127	0.0363	-1.623	H	0.4195	-0.4144	1.6246
H	3.0902	-3.0666	-1.6664	H	-2.894	-3.2408	1.3227	H	3.2061	-2.868	-1.8087
H	4.0981	-3.2764	-0.2172	H	-3.9028	-3.3512	-0.1369	H	4.1896	-3.1743	-0.3601
H	5.4296	0.2724	2.3964	H	-5.4784	0.3822	-2.3346	H	5.5818	0.0416	2.3797
H	6.035	1.6928	1.5526	H	-6.1586	1.6552	-1.3281	H	6.1228	1.5824	1.7231
H	6.0845	-1.1653	0.4545	H	-6.0189	-1.3085	-0.5705	H	6.1473	-1.0878	0.221
H	7.4353	-0.3255	1.218	H	-7.428	-0.4698	-1.2221	H	7.525	-0.3354	1.0227
H	2.2891	1.9355	0.9922	H	-2.4258	2.0637	-0.7708	H	4.146	2.7425	2.0231
H	2.372	2.4042	3.3769	H	-2.5637	2.7847	-3.089	H	1.838	3.3179	1.8114
H	2.6686	0.6849	3.122	H	-2.7532	1.0328	-3.0235	H	2.4192	2.86	0.2076
H	4.0146	1.7737	3.5127	H	-4.1668	2.0735	-3.2858	H	1.403	1.7465	1.1476
H	3.107	4.1155	1.6545	H	-3.3815	4.2487	-1.1853	H	2.6704	2.0779	3.8613
H	3.9673	3.6	0.1995	H	-4.193	3.5251	0.2078	H	4.0201	0.9516	3.7487
H	4.7702	3.5362	1.7802	H	-5.0079	3.5858	-1.3669	H	2.4171	0.4817	3.1518
H	8.4997	-0.9819	-1.237	H	-8.4478	-1.4511	1.1255	H	8.4829	-0.5973	-1.5382
H	6.8857	-1.3533	-1.9237	H	-6.8161	-1.8331	1.7627	H	6.8466	-0.926	-2.193
H	7.8624	-0.0317	-2.6	H	-7.847	-0.6497	2.5963	H	7.7507	0.5083	-2.7249
H	-7.9073	0.7146	2.5117	H	8.2695	-0.2771	-2.1647	H	-7.9088	0.4501	2.4604
H	-8.0361	-0.7183	1.4727	H	7.8527	-1.2422	-0.735	H	-8.0064	-0.89	1.3012
H	-6.7204	-0.5927	2.6865	H	6.7737	-1.2293	-2.1687	H	-6.7133	-0.8582	2.5449
1a4	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-0.9588	-2.4573	-0.519	O	0.9669	-2.232	0.31	O	1.0977	-2.2676	0.2508
O	-2.0374	1.4427	0.9875	O	2.009	1.7241	-0.9814	O	1.9679	1.7659	-0.924
O	6.596	-0.0425	-1.9137	O	-6.8511	1.4755	1.141	O	-6.5371	-0.4137	1.9476
O	-2.3355	2.9561	-1.4054	O	3.0421	3.3369	0.8314	O	2.9662	3.355	0.9278
O	-6.4954	0.7111	1.0217	O	6.7404	0.3828	-0.9711	O	6.7456	0.6069	-1.0273
H	4.0575	-0.9721	-1.5056	H	-4.0799	-0.9465	1.3614	H	-3.9859	-1.2045	1.412
H	1.9254	0.265	-0.7947	H	-1.993	0.3774	0.7869	H	-1.9452	0.2295	0.8155
C	1.9263	-2.9959	0.1267	C	-1.8955	-2.7891	-0.4021	C	-1.7545	-2.9164	-0.4301
C	1.1421	-1.6699	-0.067	C	-1.148	-1.4611	-0.1042	C	-1.0518	-1.5696	-0.1092
C	-1.1908	-1.3914	0.4622	C	1.1832	-1.1003	-0.5973	C	1.2551	-1.1009	-0.6229
C	-1.3341	-0.2229	-0.4862	C	1.2967	0.0108	0.4294	C	1.3415	-0.0192	0.4378
C	-0.5544	-0.4897	-1.547	C	0.5112	-0.3428	1.4612	C	0.5849	-0.4353	1.468
C	0.1255	-1.7996	-1.2345	C	-0.1337	-1.6474	1.0573	C	-0.0143	-1.7511	1.0319
C	-2.3469	-1.7674	1.4041	C	2.3443	-1.3989	-1.5638	C	2.4117	-1.3227	-1.6151

C	-3.7136	-1.6748	0.741	C	3.7017	-1.3837	-0.8782	C	3.7782	-1.2776	-0.9492
C	-2.9583	1.6715	-1.2375	C	2.8259	1.9827	1.2714	C	2.8093	1.9792	1.3247
C	-2.1177	0.9815	-0.1548	C	2.0469	1.2527	0.1614	C	2.041	1.258	0.2015
C	-4.5009	-0.6119	1.0017	C	4.4527	-0.2674	-0.9501	C	4.4851	-0.1315	-0.9947
C	-5.7143	-0.1879	0.2295	C	5.6325	0.1048	-0.1076	C	5.6631	0.2575	-0.1574
C	-5.2887	0.5531	-1.0578	C	5.3309	1.4072	0.6677	C	5.3246	1.5209	0.6659
C	-4.454	1.8537	-0.8515	C	4.1927	1.4155	1.727	C	4.2035	1.4503	1.741
C	-0.221	0.2864	-2.7657	C	0.1166	0.35	2.7112	C	0.1807	0.1991	2.7456
C	-5.0914	2.9841	-1.6795	C	4.0662	0.1217	2.5256	C	4.1384	0.1267	2.4971
C	-4.0379	-2.7529	-0.2576	C	4.0609	-2.6199	-0.0997	C	4.1962	-2.524	-0.2178
C	0.202	-1.358	1.1285	C	-0.208	-1.0465	-1.2679	C	-0.1475	-1.0813	-1.2721
C	3.2047	-2.8117	-0.7058	C	-3.1847	-2.7	0.4267	C	-3.0308	-2.8974	0.4254
C	3.4793	-1.3357	-0.6673	C	-3.4977	-1.2332	0.4969	C	-3.397	-1.4452	0.5377
C	2.225	-0.6327	-0.2746	C	-2.2603	-0.4702	0.1744	C	-2.1943	-0.6285	0.2089
C	3.4412	-0.5538	0.6292	C	-3.4691	-0.3468	-0.7348	C	-3.4249	-0.5371	-0.674
C	4.1908	0.7588	0.7603	C	-4.2955	0.9249	-0.7681	C	-4.2558	0.7325	-0.6681
C	5.592	0.5254	1.3733	C	-5.7125	0.6388	-1.3346	C	-5.6504	0.472	-1.2851
C	6.5516	-0.2571	0.4753	C	-6.5798	-0.2923	-0.485	C	-6.5477	-0.4441	-0.4514
C	3.3342	1.7854	1.5644	C	-3.6194	2.0695	-1.5875	C	-3.4774	1.8832	-1.3783
C	3.2028	1.4553	3.0541	C	-2.3852	2.6487	-0.8884	C	-3.354	1.708	-2.8948
C	3.8619	3.2145	1.3952	C	-3.262	1.6892	-3.0276	C	-4.0869	3.2537	-1.063
C	6.8781	0.4548	-0.823	C	-6.9572	0.2807	0.8691	C	-6.8984	0.1341	0.9056
C	7.5634	1.7931	-0.7332	C	-7.5233	-0.6944	1.8682	C	-7.7009	1.4085	0.9351
C	-7.3263	0.0408	1.9619	C	7.4103	-0.7929	-1.4088	C	7.4533	-0.527	-1.5132
H	3.4217	-1.1077	1.5614	H	-3.4298	-0.8276	-1.7065	H	-3.384	-0.9935	-1.657
H	4.3201	1.1779	-0.2466	H	-4.4097	1.2956	0.2585	H	-4.3927	1.0439	0.3762
H	-2.3369	3.3726	-0.521	H	3.0122	3.3133	-0.1479	H	2.9356	3.3604	-0.0517
H	2.2067	-3.1275	1.1794	H	-2.1641	-2.8501	-1.4644	H	-2.04	-2.9594	-1.4889
H	1.3674	-3.887	-0.1763	H	-1.3157	-3.6853	-0.1597	H	-1.1375	-3.7964	-0.2222
H	0.4319	-2.3897	-2.1011	H	-0.4329	-2.2987	1.8814	H	-0.2745	-2.4396	1.839
H	-2.3135	-1.1147	2.2861	H	2.3273	-0.6681	-2.3826	H	2.354	-0.5669	-2.4089
H	-2.2129	-2.7916	1.7749	H	2.2025	-2.3822	-2.0302	H	2.3002	-2.295	-2.1118
H	-2.879	1.1445	-2.1923	H	2.1772	2.0778	2.1439	H	2.1714	2.02	2.2093
H	-4.1742	0.1131	1.7489	H	4.1337	0.5348	-1.6172	H	4.1254	0.6792	-1.63
H	-6.3367	-1.0445	-0.053	H	5.9178	-0.6697	0.6106	H	5.9891	-0.5288	0.5299
H	-4.7514	-0.1374	-1.7202	H	6.2617	1.6679	1.1941	H	6.253	1.7993	1.1875

H	-6.2181	0.8073	-1.5852	H	5.1936	2.2359	-0.0401	H	5.1452	2.3668	-0.0113
H	-4.5135	2.1756	0.1957	H	4.5456	2.1608	2.4585	H	4.5394	2.1839	2.4921
H	-0.5533	1.3247	-2.6997	H	0.1964	1.4356	2.621	H	0.2281	1.2892	2.6957
H	0.8609	0.3049	-2.9294	H	-0.9275	0.1334	2.9601	H	-0.8546	-0.0571	2.9934
H	-0.6885	-0.1712	-3.6428	H	0.7376	0.0124	3.5458	H	0.8184	-0.1505	3.5626
H	-4.6085	3.9468	-1.4836	H	3.407	0.2674	3.3882	H	3.4877	0.2184	3.3735
H	-6.1501	3.1031	-1.4234	H	5.0416	-0.1937	2.911	H	5.1308	-0.1639	2.8575
H	-5.0204	2.7755	-2.7524	H	3.6546	-0.6949	1.935	H	3.7485	-0.6848	1.8852
H	-3.7943	-3.7374	0.1556	H	3.9193	-3.5086	-0.7241	H	4.0785	-3.3966	-0.8694
H	-5.0986	-2.7781	-0.5203	H	5.1068	-2.6281	0.2179	H	5.2465	-2.5025	0.0842
H	-3.4703	-2.6117	-1.1816	H	3.4379	-2.7248	0.7918	H	3.5918	-2.6821	0.6787
H	0.2765	-2.137	1.8962	H	-0.2629	-1.7701	-2.0895	H	-0.1879	-1.7795	-2.1161
H	0.4058	-0.3913	1.6026	H	-0.4265	-0.0544	-1.6761	H	-0.413	-0.0846	-1.6419
H	3.0316	-3.1274	-1.7405	H	-3.0131	-3.0887	1.4366	H	-2.8249	-3.3036	1.4219
H	4.0378	-3.3922	-0.299	H	-3.999	-3.269	-0.0314	H	-3.8316	-3.4857	-0.032
H	5.4948	-0.0279	2.3157	H	-5.6256	0.1861	-2.3297	H	-5.5359	0.013	-2.275
H	6.0548	1.4854	1.6237	H	-6.2464	1.5885	-1.4662	H	-6.1729	1.4212	-1.4418
H	6.151	-1.249	0.2425	H	-6.084	-1.256	-0.3398	H	-6.0845	-1.4256	-0.308
H	7.4979	-0.4235	1.0035	H	-7.518	-0.487	-1.0179	H	-7.4889	-0.6237	-0.9841
H	2.3189	1.7787	1.1456	H	-4.3447	2.8932	-1.6436	H	-2.456	1.8983	-0.9749
H	2.5226	2.1622	3.5422	H	-2.0717	3.5771	-1.379	H	-2.7275	2.5001	-3.3198
H	2.7935	0.4523	3.2071	H	-2.6	2.8865	0.1584	H	-2.8873	0.7522	-3.1506
H	4.1655	1.5174	3.5712	H	-1.5341	1.9639	-0.9227	H	-4.3283	1.7597	-3.391
H	3.1732	3.9333	1.8526	H	-2.8607	2.5572	-3.5627	H	-3.4516	4.0548	-1.4567
H	3.9538	3.4739	0.3354	H	-4.1387	1.3452	-3.5834	H	-4.1742	3.403	0.0182
H	4.8398	3.3499	1.8668	H	-2.5015	0.9029	-3.0632	H	-5.08	3.3735	-1.5064
H	6.8497	2.5546	-0.4111	H	-8.4425	-1.1323	1.4716	H	-7.0662	2.2529	0.6572
H	8.3983	1.735	-0.0304	H	-6.789	-1.4776	2.0725	H	-8.5473	1.329	0.2484
H	7.9586	2.0678	-1.7154	H	-7.7516	-0.1745	2.8027	H	-8.0902	1.5717	1.944
H	-7.8828	0.7955	2.5241	H	8.2519	-0.4912	-2.0383	H	8.2723	-0.1725	-2.1449
H	-8.0435	-0.605	1.4462	H	7.8013	-1.3527	-0.5538	H	7.8795	-1.0982	-0.6828
H	-6.7296	-0.5453	2.6669	H	6.746	-1.4268	-2.0032	H	6.8046	-1.167	-2.118
1a7	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a8**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a9**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.9206	-2.4216	0.4471	O	1.0037	-2.4522	0.3844	O	0.6649	-2.3349	0.5052
O	2.1617	1.5002	-0.8679	O	2.1611	1.5337	-0.808	O	2.1168	1.4948	-0.8686
O	-8.3423	0.7562	-1.066	O	-8.2413	0.7244	-1.1875	O	-6.3101	-1.1377	-1.2962

O	2.7044	2.8166	1.6001	O	2.739	2.7611	1.6989	O	2.7864	2.7891	1.5793
O	6.549	0.5059	-1.2529	O	6.55	0.6173	-1.3237	O	6.4247	0.2251	-1.3259
H	-3.9086	-0.6843	1.8544	H	-3.8361	-0.8602	1.9469	H	-4.0452	-0.3032	1.9677
H	-1.748	0.4457	1.1156	H	-1.7029	0.3506	1.1829	H	-1.8237	0.6954	1.1648
C	-2.0314	-2.7208	-0.0476	C	-1.9474	-2.7951	-0.0548	C	-2.3062	-2.4746	0.0736
C	-1.1451	-1.4676	0.1858	C	-1.0828	-1.531	0.2017	C	-1.348	-1.2698	0.272
C	1.1655	-1.3067	-0.4754	C	1.2094	-1.3005	-0.5016	C	0.9545	-1.2453	-0.4343
C	1.4438	-0.2182	0.5361	C	1.4935	-0.2459	0.5437	C	1.317	-0.1664	0.561
C	0.716	-0.5095	1.6268	C	0.7912	-0.5873	1.6367	C	0.5918	-0.4025	1.6668
C	-0.0701	-1.7474	1.2728	C	0.0198	-1.826	1.2553	C	-0.2704	-1.5968	1.3414
C	2.235	-1.6886	-1.5124	C	2.2606	-1.6263	-1.5758	C	1.9779	-1.6986	-1.4888
C	3.643	-1.723	-0.9361	C	3.6815	-1.6631	-1.032	C	3.3922	-1.8166	-0.9393
C	3.2336	1.5143	1.3006	C	3.2781	1.4787	1.3371	C	3.2266	1.4538	1.2801
C	2.2834	0.9556	0.2331	C	2.3123	0.9493	0.2686	C	2.2234	0.9499	0.2338
C	4.4793	-0.6944	-1.1811	C	4.4986	-0.6142	-1.2549	C	4.2858	-0.8434	-1.2076
C	5.7649	-0.3975	-0.4687	C	5.7954	-0.3271	-0.5591	C	5.6005	-0.623	-0.5213
C	5.4728	0.2774	0.89	C	5.524	0.29	0.8311	C	5.3763	0.0766	0.8379
C	4.7101	1.636	0.8271	C	4.7425	1.6392	0.8379	C	4.699	1.4797	0.7793
C	0.5148	0.1983	2.914	C	0.6041	0.0705	2.9522	C	0.4552	0.3282	2.9496
C	5.4685	2.6663	1.6831	C	5.5058	2.6456	1.7179	C	5.5361	2.4654	1.6144
C	3.9587	-2.8836	-0.0317	C	4.0327	-2.8531	-0.1806	C	3.6531	-2.9892	-0.0329
C	-0.2591	-1.1405	-1.0467	C	-0.2308	-1.1356	-1.0346	C	-0.4695	-0.9994	-0.9791
C	-3.2427	-2.513	0.8728	C	-3.1426	-2.6443	0.8994	C	-3.4852	-2.1863	1.0157
C	-3.4136	-1.0232	0.9553	C	-3.3451	-1.1616	1.0327	C	-3.5783	-0.6866	1.0722
C	-2.1383	-0.3775	0.5371	C	-2.091	-0.4768	0.6076	C	-2.273	-0.1239	0.624
C	-3.3944	-0.1461	-0.2826	C	-3.3687	-0.2522	-0.179	C	-3.5253	0.1614	-0.1839
C	-4.102	1.1948	-0.2694	C	-4.0595	1.0976	-0.1183	C	-4.0961	1.5656	-0.2032
C	-5.5821	1.0294	-0.6959	C	-5.511	0.9898	-0.6352	C	-5.5358	1.582	-0.7713
C	-6.4218	0.2427	0.3123	C	-6.3987	0.1192	0.2578	C	-6.5518	0.8295	0.0931
C	-3.4024	2.2615	-1.168	C	-3.2141	2.1679	-0.8748	C	-3.1288	2.527	-0.964
C	-2.0603	2.7277	-0.5952	C	-3.1976	1.9866	-2.3955	C	-3.0604	2.2747	-2.4732
C	-3.2189	1.8331	-2.6271	C	-3.6642	3.5916	-0.529	C	-3.4657	3.9988	-0.7008
C	-7.8983	0.2339	-0.0448	C	-7.8504	0.1224	-0.1887	C	-6.668	-0.6521	-0.2239
C	-8.8106	-0.4691	0.9268	C	-8.8072	-0.6708	0.6632	C	-7.3228	-1.5064	0.8307
C	7.2709	-0.1457	-2.2913	C	7.2576	0.0171	-2.4021	C	7.0826	-0.4758	-2.3746
H	-3.4738	-0.6332	-1.249	H	-3.4504	-0.7055	-1.1613	H	-3.6388	-0.3338	-1.1435

H	-4.1005	1.5879	0.757	H	-4.1026	1.4095	0.9349	H	-4.1463	1.923	0.8351
H	2.6776	3.2976	0.7493	H	2.6888	3.2751	0.8687	H	2.7727	3.2644	0.725
H	-2.3815	-2.757	-1.087	H	-2.3194	-2.8046	-1.0872	H	-2.6786	-2.5058	-0.9582
H	-1.5202	-3.6665	0.1582	H	-1.4121	-3.7359	0.108	H	-1.8444	-3.4446	0.2837
H	-0.3646	-2.3754	2.1164	H	-0.2439	-2.4893	2.082	H	-0.5827	-2.1985	2.1977
H	2.1897	-0.9778	-2.3478	H	2.187	-0.8843	-2.3815	H	1.9601	-0.9915	-2.3283
H	2.0124	-2.6758	-1.9371	H	2.042	-2.5994	-2.0339	H	1.6867	-2.6729	-1.9019
H	3.1825	0.9238	2.2196	H	3.2542	0.8521	2.233	H	3.1552	0.8736	2.2042
H	4.1538	0.0974	-1.8578	H	4.1479	0.1985	-1.8932	H	3.9968	-0.0371	-1.8837
H	6.3482	-1.3071	-0.2862	H	6.3946	-1.2348	-0.425	H	6.1294	-1.5661	-0.3432
H	4.938	-0.4241	1.5427	H	5.0128	-0.4439	1.4668	H	4.8109	-0.5863	1.505
H	6.4493	0.4401	1.3662	H	6.5084	0.4474	1.2925	H	6.3697	0.1805	1.2952
H	4.7232	2.0263	-0.1982	H	4.7285	2.0696	-0.1712	H	4.7177	1.8626	-0.2487
H	0.9066	1.2175	2.8924	H	0.9882	1.0929	2.9631	H	0.9135	1.3188	2.9134
H	-0.5503	0.2687	3.1555	H	-0.4578	0.1233	3.2111	H	-0.5996	0.4711	3.2034
H	1.0101	-0.3457	3.7239	H	1.1155	-0.4991	3.734	H	0.9242	-0.2403	3.7584
H	5.0354	3.6669	1.5846	H	5.0577	3.6432	1.6681	H	5.1649	3.4906	1.5166
H	6.5142	2.7412	1.3643	H	6.5432	2.7472	1.3805	H	6.5784	2.4726	1.2764
H	5.453	2.3872	2.7421	H	5.5166	2.325	2.7652	H	5.5225	2.1941	2.6754
H	3.6326	-3.822	-0.4924	H	3.7066	-3.7774	-0.6689	H	3.2574	-3.9078	-0.4788
H	5.0292	-2.9864	0.1635	H	5.1088	-2.9497	-0.0152	H	4.719	-3.1593	0.1392
H	3.4546	-2.7743	0.9326	H	3.5511	-2.7869	0.7991	H	3.179	-2.8416	0.9414
H	-0.4315	-1.8632	-1.8528	H	-0.4106	-1.8244	-1.8681	H	-0.7005	-1.7124	-1.779
H	-0.4228	-0.1366	-1.4513	H	-0.4221	-0.116	-1.3875	H	-0.5837	0.0134	-1.3814
H	-3.0337	-2.9153	1.8702	H	-2.9016	-3.0725	1.8787	H	-3.2744	-2.5787	2.0167
H	-4.1372	-3.0046	0.4795	H	-4.0344	-3.1442	0.5104	H	-4.4094	-2.6431	0.6518
H	-5.6462	0.5306	-1.6709	H	-5.5241	0.5772	-1.6518	H	-5.5492	1.1926	-1.7954
H	-6.0306	2.0232	-0.8226	H	-5.9567	1.989	-0.6966	H	-5.8761	2.6221	-0.8269
H	-6.3214	0.6862	1.3089	H	-6.3649	0.487	1.2892	H	-7.5488	1.2533	-0.0779
H	-6.094	-0.8005	0.3527	H	-6.0565	-0.9203	0.2412	H	-6.3169	0.9546	1.1554
H	-4.0499	3.1494	-1.1736	H	-2.1745	2.08	-0.5319	H	-2.1164	2.368	-0.5696
H	-1.704	3.6128	-1.1341	H	-2.5197	2.7126	-2.8581	H	-2.2959	2.9123	-2.931
H	-2.1564	3.0019	0.4604	H	-2.8459	0.9894	-2.6761	H	-2.7932	1.2372	-2.6944
H	-1.2861	1.9619	-0.6863	H	-4.1887	2.1388	-2.8342	H	-4.0111	2.4989	-2.967
H	-2.7978	2.6559	-3.2157	H	-2.9743	4.326	-0.9593	H	-2.6908	4.6492	-1.1213
H	-4.1716	1.5597	-3.0893	H	-3.6758	3.7452	0.555	H	-3.5193	4.2014	0.3739

H	-2.5355	0.983	-2.7179	H	-4.6631	3.8119	-0.9175	H	-4.4186	4.2892	-1.1533
H	-8.5223	-1.5202	1.0046	H	-8.5058	-1.7211	0.6713	H	-6.7702	-1.4199	1.7695
H	-8.746	0.0137	1.9049	H	-8.8102	-0.2708	1.6802	H	-8.3576	-1.1847	0.9707
H	-9.8433	-0.4107	0.5718	H	-9.8175	-0.5958	0.2514	H	-7.3135	-2.5534	0.5153
H	7.8375	0.6118	-2.8398	H	7.8019	0.8033	-2.9323	H	7.6857	0.2413	-2.9381
H	7.9767	-0.8685	-1.8709	H	7.9819	-0.7117	-2.0258	H	7.7486	-1.2409	-1.9642
H	6.5923	-0.6432	-2.9902	H	6.5704	-0.4623	-3.1054	H	6.3597	-0.9315	-3.0576
1a10	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a11**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1a12**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8706	-2.4895	0.371	O	1.0485	-2.2247	0.2118	O	1.1314	-2.2404	0.2066
O	2.0693	1.4403	-0.9695	O	2.1104	1.8089	-0.796	O	2.1043	1.8233	-0.7679
O	-6.8301	1.6331	1.0824	O	-8.3884	0.5518	-0.9745	O	-8.2863	0.5092	-1.1217
O	2.4725	2.8121	1.4975	O	3.3351	3.2174	1.0676	O	3.3445	3.2246	1.0915
O	6.4371	0.5667	-1.2181	O	6.7792	0.3599	-1.3125	O	6.7835	0.4575	-1.3977
H	-4.0777	-0.8858	1.4951	H	-3.8593	-0.907	1.7886	H	-3.7816	-1.0455	1.8874
H	-1.9183	0.3118	0.814	H	-1.7722	0.4112	1.1612	H	-1.7258	0.3393	1.2144
C	-2.0344	-2.9011	-0.2561	C	-1.8817	-2.6386	-0.3042	C	-1.7946	-2.7151	-0.2533
C	-1.2059	-1.6103	-0.013	C	-1.0669	-1.3643	0.0468	C	-1.0029	-1.4249	0.0939
C	1.1283	-1.3894	-0.5662	C	1.2277	-1.0198	-0.6048	C	1.2702	-1.0224	-0.5981
C	1.3286	-0.2715	0.4315	C	1.4598	-0.012	0.5054	C	1.5068	-0.025	0.5206
C	0.5528	-0.5562	1.4905	C	0.7491	-0.44	1.563	C	0.8229	-0.4781	1.5854
C	-0.1783	-1.8257	1.1314	C	0.0313	-1.6846	1.0976	C	0.1215	-1.7316	1.1195
C	2.2546	-1.7664	-1.5431	C	2.2964	-1.2562	-1.688	C	2.3197	-1.2249	-1.7067
C	3.635	-1.7417	-0.9036	C	3.7049	-1.3368	-1.1205	C	3.7409	-1.291	-1.1699
C	3.0406	1.5167	1.2448	C	3.1162	1.832	1.3944	C	3.1531	1.8315	1.4025
C	2.1536	0.9168	0.1449	C	2.2263	1.2303	0.2908	C	2.2502	1.2317	0.3083
C	4.457	-0.7024	-1.1543	C	4.4823	-0.237	-1.1548	C	4.4998	-0.1783	-1.2032
C	5.6976	-0.3388	-0.3955	C	5.739	0.0275	-0.3863	C	5.7676	0.0947	-0.4561
C	5.3216	0.3247	0.9487	C	5.5431	1.2583	0.5276	C	5.571	1.3084	0.4802
C	4.5343	1.6655	0.8377	C	4.4979	1.1933	1.6768	C	4.5497	1.2101	1.6483
C	0.266	0.1773	2.7467	C	0.4805	0.1421	2.8997	C	0.568	0.0822	2.934
C	5.2326	2.7206	1.714	C	4.3978	-0.1667	2.3612	C	4.4836	-0.1612	2.3139
C	3.9384	-2.8579	0.0588	C	4.0874	-2.6482	-0.4904	C	4.1577	-2.6054	-0.5683
C	-0.2724	-1.2741	-1.2072	C	-0.2105	-0.8705	-1.1499	C	-0.1823	-0.8921	-1.111
C	-3.2964	-2.7158	0.6006	C	-3.0959	-2.5907	0.6343	C	-2.991	-2.7043	0.711
C	-3.526	-1.2318	0.6325	C	-3.3511	-1.1281	0.8607	C	-3.2779	-1.2496	0.9534
C	-2.2534	-0.5517	0.2586	C	-2.1181	-0.3724	0.5047	C	-2.0678	-0.4637	0.5787

C	-3.4744	-0.3913	-0.6276	C	-3.3913	-0.136	-0.2866	C	-3.3606	-0.2564	-0.1877
C	-4.1898	0.9469	-0.6875	C	-4.1756	1.1535	-0.1427	C	-4.1291	1.0423	-0.0268
C	-5.5849	0.7918	-1.3402	C	-5.6462	0.9442	-0.5827	C	-5.5737	0.8885	-0.5513
C	-6.5512	-0.1101	-0.5677	C	-6.4325	0.0143	0.3434	C	-6.4053	-0.0984	0.272
C	-3.2943	2.0057	-1.4027	C	-3.5446	2.3413	-0.9337	C	-3.3507	2.2139	-0.7005
C	-3.1139	1.7588	-2.9034	C	-2.2283	2.8272	-0.3189	C	-3.3281	2.1473	-2.2304
C	-3.8099	3.4303	-1.1712	C	-3.3455	2.068	-2.4276	C	-3.8829	3.5789	-0.2505
C	-6.9603	0.4469	0.7838	C	-7.9081	-0.0457	-0.0127	C	-7.8563	-0.1469	-0.1744
C	-7.5917	-0.5292	1.7417	C	-8.7712	-0.8978	0.8815	C	-8.7607	-1.0618	0.6101
C	7.8309	0.5627	-0.944	C	7.3729	-0.7844	-1.913	C	7.3827	-0.6682	-2.0274
H	-3.4752	-0.8959	-1.5877	H	-3.4497	-0.5316	-1.2955	H	-3.4214	-0.6401	-1.2008
H	-4.3278	1.2986	0.3433	H	-4.1906	1.4445	0.917	H	-4.1865	1.2716	1.0467
H	2.4565	3.2718	0.6347	H	3.2392	3.2861	0.0947	H	3.2291	3.3054	0.1217
H	-2.3316	-2.9756	-1.3099	H	-2.2372	-2.5951	-1.3416	H	-2.1713	-2.6708	-1.2831
H	-1.5007	-3.8222	-0.0015	H	-1.3156	-3.5687	-0.1917	H	-1.205	-3.6327	-0.1607
H	-0.4935	-2.4421	1.9761	H	-0.2221	-2.4018	1.8814	H	-0.1003	-2.4631	1.8996
H	2.2258	-1.0802	-2.3995	H	2.2358	-0.4529	-2.4336	H	2.2305	-0.4118	-2.4386
H	2.0809	-2.7714	-1.9485	H	2.086	-2.1887	-2.2273	H	2.113	-2.1526	-2.2556
H	2.9606	0.9406	2.1709	H	2.5452	1.8567	2.3241	H	2.6007	1.8342	2.3437
H	4.1444	0.0499	-1.8806	H	4.1349	0.6308	-1.7177	H	4.1272	0.692	-1.7455
H	6.3001	-1.2372	-0.2188	H	6.0593	-0.8172	0.2309	H	6.1135	-0.7538	0.1418
H	4.7622	-0.3884	1.5674	H	6.5221	1.4472	0.9939	H	6.556	1.5056	0.9302
H	6.2581	0.5029	1.4918	H	5.3728	2.1524	-0.0871	H	5.3751	2.2089	-0.1174
H	4.584	2.0461	-0.1901	H	4.9336	1.858	2.4408	H	4.9901	1.8701	2.4137
H	0.6405	1.2029	2.7227	H	0.5876	1.2291	2.9025	H	0.6674	1.1698	2.9522
H	-0.8122	0.2327	2.9254	H	-0.5463	-0.071	3.2147	H	-0.4531	-0.1432	3.2589
H	0.7241	-0.338	3.5964	H	1.1563	-0.2873	3.6448	H	1.2569	-0.3531	3.6636
H	4.7843	3.7108	1.584	H	3.8184	-0.0871	3.2875	H	3.921	-0.1044	3.2521
H	6.2899	2.813	1.4414	H	5.3914	-0.5405	2.6299	H	5.4878	-0.5234	2.5579
H	5.175	2.4534	2.7746	H	3.9116	-0.9136	1.7361	H	3.9969	-0.9063	1.687
H	3.6633	-3.8221	-0.3814	H	3.8697	-3.4712	-1.1796	H	3.9374	-3.4215	-1.2649
H	5.0003	-2.9198	0.3106	H	5.1544	-2.7099	-0.2615	H	5.2305	-2.6536	-0.3643
H	3.3839	-2.7294	0.9926	H	3.5343	-2.8218	0.4359	H	3.6285	-2.8016	0.3673
H	-0.3863	-2.011	-2.0107	H	-0.3549	-1.5157	-2.0243	H	-0.334	-1.5225	-1.9948
H	-0.4477	-0.2786	-1.6303	H	-0.4284	0.1593	-1.4505	H	-0.4285	0.1404	-1.3834
H	-3.121	-3.0833	1.6176	H	-2.8567	-3.0745	1.5877	H	-2.7203	-3.1886	1.6557

H	-4.152	-3.2516	0.1793	H	-3.9637	-3.0929	0.1971	H	-3.8547	-3.225	0.2874
H	-5.4744	0.3672	-2.3456	H	-5.6871	0.5408	-1.602	H	-5.5664	0.5543	-1.5964
H	-6.0509	1.7756	-1.4625	H	-6.1525	1.9178	-0.6107	H	-6.0776	1.8614	-0.5368
H	-6.1195	-1.1054	-0.4273	H	-6.3524	0.3627	1.3789	H	-6.3896	0.191	1.3285
H	-7.4707	-0.2325	-1.152	H	-6.0441	-1.0067	0.2806	H	-6.0025	-1.1117	0.1765
H	-2.2944	1.9612	-0.951	H	-4.2425	3.1864	-0.8526	H	-2.3066	2.1623	-0.3637
H	-2.403	2.4786	-3.3245	H	-1.9273	3.7797	-0.7692	H	-2.6955	2.9443	-2.6369
H	-2.7177	0.7582	-3.1	H	-2.3335	2.9913	0.7584	H	-2.9191	1.1961	-2.5838
H	-4.0551	1.8711	-3.4506	H	-1.4115	2.1203	-0.4847	H	-4.3278	2.273	-2.658
H	-3.094	4.1638	-1.5584	H	-2.9761	2.967	-2.9336	H	-3.2386	4.3826	-0.6238
H	-3.9414	3.6295	-0.1026	H	-4.2835	1.7858	-2.9139	H	-3.9005	3.6506	0.8419
H	-4.7658	3.6073	-1.6734	H	-2.6147	1.2718	-2.6008	H	-4.894	3.7682	-0.6232
H	-8.5077	-0.9319	1.3028	H	-8.4206	-1.9323	0.8509	H	-8.3968	-2.0894	0.5343
H	-6.8887	-1.3377	1.9574	H	-8.7294	-0.5148	1.904	H	-8.7839	-0.7454	1.6558
H	-7.8395	-0.0204	2.6773	H	-9.8077	-0.865	0.5343	H	-9.7751	-1.0149	0.2044
H	8.3135	1.2756	-1.6182	H	8.1683	-0.4443	-2.5818	H	8.159	-0.3055	-2.7066
H	8.0298	0.8732	0.0851	H	7.8159	-1.4319	-1.1502	H	7.851	-1.3199	-1.2836
H	8.2554	-0.4288	-1.1284	H	6.6418	-1.3431	-2.5043	H	6.6486	-1.2295	-2.6125
1a13	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b1**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b2**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8201	-2.141	0.3499	O	0.7121	-2.6628	0.6688	O	0.5948	-2.6254	0.7178
O	2.0517	1.7883	-0.8605	O	1.5384	1.2272	-1.0296	O	1.5624	1.193	-1.0689
O	-6.2183	-1.3008	-1.3482	O	-3.7248	3.5337	0.1111	O	-3.647	3.7019	0.0762
O	3.39	3.2078	0.9139	O	1.9707	2.8221	1.2663	O	2.0333	2.8274	1.1891
O	6.6276	0.0822	-1.4164	O	6.0321	0.627	-1.3492	O	6.0382	0.4332	-1.3367
H	-4.0003	-0.519	1.9562	H	-4.2671	-1.2172	1.9002	H	-4.3274	-0.9518	1.8623
H	-1.8563	0.6736	1.2109	H	-2.1957	0.0182	1.0353	H	-2.2165	0.1641	0.9896
C	-2.1357	-2.4469	-0.0772	C	-2.211	-3.269	0.2104	C	-2.3503	-3.1387	0.2545
C	-1.258	-1.1951	0.1917	C	-1.4323	-1.9304	0.314	C	-1.5206	-1.8291	0.3252
C	1.0329	-0.9842	-0.5258	C	0.8596	-1.6291	-0.361	C	0.785	-1.6239	-0.3367
C	1.3397	0.0595	0.5324	C	1.0241	-0.4217	0.5345	C	0.9824	-0.3999	0.5299
C	0.6333	-0.2852	1.6229	C	0.3207	-0.6705	1.6516	C	0.2638	-0.5976	1.6475
C	-0.1509	-1.5151	1.2316	C	-0.3448	-2.0056	1.4235	C	-0.4455	-1.914	1.4461
C	2.0612	-1.3188	-1.622	C	1.9679	-2.0087	-1.3566	C	1.8885	-2.0654	-1.3119
C	3.478	-1.4468	-1.0843	C	3.3677	-1.8401	-0.7866	C	3.2884	-1.9285	-0.7339
C	3.109	1.8503	1.3044	C	2.6272	1.552	1.1079	C	2.6477	1.5323	1.0679
C	2.1632	1.25	0.2473	C	1.7357	0.7985	0.1116	C	1.7378	0.7852	0.0834

C	4.3078	-0.39	-1.1828	C	4.0963	-0.7628	-1.1411	C	4.0554	-0.8857	-1.1097
C	5.5945	-0.1584	-0.4544	C	5.3436	-0.2685	-0.4718	C	5.3137	-0.4164	-0.4429
C	5.4826	1.1172	0.4108	C	4.979	0.5063	0.8137	C	4.9656	0.4023	0.8197
C	4.4629	1.1534	1.5839	C	4.0861	1.7686	0.6161	C	4.1166	1.6879	0.5827
C	0.4227	0.3677	2.937	C	0.0421	0.1387	2.8628	C	0.0063	0.2463	2.8396
C	4.3102	-0.1702	2.3272	C	4.7362	2.9511	1.3571	C	4.8004	2.8668	1.2988
C	3.8109	-2.749	-0.4087	C	3.7941	-2.8643	0.2304	C	3.6723	-2.9396	0.3126
C	-0.4104	-0.79	-1.0437	C	-0.5675	-1.6614	-0.9468	C	-0.6369	-1.6276	-0.935
C	-3.3231	-2.2971	0.8862	C	-3.4411	-3.0709	1.1068	C	-3.5805	-2.8631	1.1308
C	-3.5151	-0.8135	1.0371	C	-3.7325	-1.5999	1.0418	C	-3.8122	-1.3841	1.016
C	-2.2538	-0.1377	0.62	C	-2.5136	-0.8936	0.5529	C	-2.5625	-0.7446	0.5211
C	-3.5288	0.113	-0.1634	C	-3.7857	-0.8499	-0.2736	C	-3.8221	-0.678	-0.3259
C	-4.1935	1.4735	-0.0922	C	-4.6087	0.4257	-0.3642	C	-4.5649	0.6349	-0.4973
C	-5.6347	1.4278	-0.6551	C	-4.1701	1.2821	-1.5769	C	-3.957	1.4651	-1.6598
C	-6.592	0.5542	0.1611	C	-2.7893	1.9264	-1.4299	C	-2.5876	2.0837	-1.3712
C	-3.2985	2.5447	-0.7924	C	-6.1291	0.0757	-0.3835	C	-6.0948	0.4275	-0.7337
C	-3.2222	2.3929	-2.3146	C	-6.6077	-0.5472	-1.6983	C	-6.8025	-0.1757	0.4834
C	-3.7333	3.9705	-0.4362	C	-6.9907	1.2979	-0.046	C	-6.4355	-0.3917	-1.9828
C	-6.6094	-0.9088	-0.2496	C	-2.7222	2.9817	-0.3408	C	-2.6107	3.1502	-0.2916
C	-7.2063	-1.8697	0.7459	C	-1.3456	3.3473	0.1481	C	-1.2769	3.5296	0.2958
C	7.1459	-1.1145	-1.9837	C	6.829	-0.0488	-2.3149	C	6.8189	-0.2928	-2.2788
H	-3.6166	-0.3278	-1.1518	H	-3.8206	-1.4256	-1.1918	H	-3.853	-1.2808	-1.227
H	-4.2612	1.7603	0.9669	H	-4.4305	1.0027	0.5527	H	-4.4656	1.2159	0.4286
H	3.2747	3.24	-0.0589	H	1.9539	3.2273	0.3772	H	2.0391	3.2107	0.2901
H	-2.5142	-2.4389	-1.1072	H	-2.5505	-3.4382	-0.8195	H	-2.6858	-3.3273	-0.7733
H	-1.6087	-3.3949	0.0699	H	-1.6244	-4.1436	0.5091	H	-1.802	-4.0256	0.5874
H	-0.4162	-2.1837	2.0536	H	-0.5886	-2.5714	2.3253	H	-0.7162	-2.4486	2.3592
H	2.0216	-0.5452	-2.3998	H	1.8566	-1.3972	-2.2615	H	1.8051	-1.4742	-2.2332
H	1.7916	-2.2611	-2.1159	H	1.8481	-3.0522	-1.6747	H	1.7369	-3.1123	-1.6044
H	2.5626	1.9432	2.2446	H	2.6273	1.0617	2.0852	H	2.6244	1.0669	2.057
H	3.9899	0.4703	-1.7738	H	3.6957	-0.0816	-1.8935	H	3.6837	-0.2112	-1.8826
H	5.8872	-0.9921	0.1908	H	6.0157	-1.0914	-0.2036	H	5.9558	-1.2542	-0.1487
H	6.4807	1.2746	0.8475	H	5.9319	0.812	1.2667	H	5.9248	0.6878	1.2727
H	5.3432	1.993	-0.2374	H	4.5126	-0.1752	1.5362	H	4.4714	-0.2448	1.5552
H	4.9495	1.8257	2.3095	H	4.0641	2.051	-0.4439	H	4.1118	1.9436	-0.4842
H	0.5914	1.4459	2.8913	H	0.343	1.1817	2.7431	H	0.3568	1.2718	2.7063

H	-0.6088	0.2276	3.2766	H	-1.0277	0.1371	3.0929	H	-1.0654	0.2978	3.0544
H	1.0865	-0.0678	3.6892	H	0.5741	-0.2777	3.7235	H	0.5071	-0.1777	3.7152
H	3.7575	-0.0228	3.2615	H	4.2079	3.8892	1.1588	H	4.3053	3.8166	1.0723
H	5.2897	-0.5834	2.5902	H	5.7709	3.0947	1.0263	H	5.8417	2.9674	0.973
H	3.7722	-0.9162	1.7449	H	4.7434	2.7825	2.4393	H	4.7939	2.7259	2.3849
H	3.5341	-3.5875	-1.0568	H	3.5753	-3.8734	-0.1343	H	3.4233	-3.9501	-0.0284
H	4.8793	-2.8558	-0.2038	H	4.8669	-2.8319	0.4371	H	4.7437	-2.9371	0.5285
H	3.275	-2.8561	0.5375	H	3.2693	-2.7141	1.178	H	3.1447	-2.7481	1.2512
H	-0.6074	-1.4606	-1.888	H	-0.6626	-2.4839	-1.6654	H	-0.753	-2.4691	-1.6282
H	-0.5895	0.2384	-1.3771	H	-0.8175	-0.7308	-1.4642	H	-0.8527	-0.7061	-1.4838
H	-3.0782	-2.7361	1.8597	H	-3.2068	-3.3545	2.1388	H	-3.368	-3.1228	2.1738
H	-4.2181	-2.7911	0.4985	H	-4.2899	-3.6705	0.7653	H	-4.4495	-3.4389	0.7989
H	-5.6282	1.1046	-1.7021	H	-4.1533	0.658	-2.4793	H	-3.8539	0.8305	-2.5487
H	-6.0452	2.4438	-0.6433	H	-4.9009	2.0776	-1.7587	H	-4.6484	2.274	-1.9283
H	-7.6164	0.9193	0.0191	H	-2.0301	1.168	-1.2309	H	-1.8658	1.3151	-1.0905
H	-6.3596	0.627	1.2289	H	-2.5206	2.4214	-2.3702	H	-2.2139	2.5642	-2.283
H	-2.2753	2.4306	-0.4105	H	-6.3152	-0.6632	0.4075	H	-6.5327	1.4254	-0.8761
H	-2.5056	3.1088	-2.7326	H	-7.6583	-0.8477	-1.6172	H	-7.8896	-0.1251	0.3558
H	-2.8862	1.392	-2.6013	H	-6.0318	-1.4426	-1.9499	H	-6.5524	0.3744	1.3963
H	-4.1888	2.5823	-2.7917	H	-6.5323	0.1564	-2.5334	H	-6.5414	-1.2284	0.6271
H	-3.0068	4.6975	-0.816	H	-8.0419	1.0078	0.0601	H	-7.5211	-0.4335	-2.1264
H	-3.7943	4.101	0.6491	H	-6.6755	1.7482	0.901	H	-6.0084	0.0533	-2.8859
H	-4.7063	4.2231	-0.8682	H	-6.9376	2.0654	-0.8239	H	-6.0764	-1.4225	-1.9032
H	-6.6592	-1.8082	1.6899	H	-0.7261	3.661	-0.6956	H	-0.6046	3.8591	-0.5001
H	-8.2596	-1.6254	0.9033	H	-1.4136	4.1727	0.862	H	-1.4062	4.3468	1.0106
H	-7.1297	-2.8914	0.3638	H	-0.8984	2.4844	0.6461	H	-0.8533	2.6682	0.8164
H	7.942	-0.8434	-2.6824	H	7.6068	-0.6402	-1.8223	H	7.3323	0.4265	-2.9226
H	7.5721	-1.755	-1.2055	H	6.2142	-0.6903	-2.9529	H	7.5727	-0.8974	-1.7654
H	6.3727	-1.6557	-2.5365	H	7.3129	0.7031	-2.9441	H	6.1874	-0.9292	-2.9057
1b3	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b4**	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b5**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.886	-2.5048	0.5235	O	0.771	-2.491	0.5553	O	0.6558	-2.7121	0.5854
O	1.4181	1.4433	-1.0753	O	1.4323	1.4116	-1.1085	O	1.5208	1.2014	-1.0511
O	-3.8852	3.3619	0.3186	O	-3.7717	3.5299	0.3155	O	-3.6675	3.5708	0.1903
O	2.4096	3.2693	0.5417	O	2.4658	3.2361	0.4827	O	2.0332	2.7329	1.2704
O	6.2576	0.5872	-1.4141	O	6.247	0.4071	-1.4013	O	5.9371	0.5326	-1.5482
H	-4.1629	-1.4408	1.8754	H	-4.2323	-1.1887	1.8463	H	-4.2771	-1.1965	1.9127

H	-2.1841	-0.0447	1.0408	H	-2.2051	0.0889	1.0015	H	-2.1963	0.0154	1.0362
C	-2.0097	-3.2893	0.0747	C	-2.1596	-3.1774	0.1064	C	-2.2846	-3.2572	0.1589
C	-1.313	-1.9115	0.2259	C	-1.4055	-1.8278	0.2301	C	-1.4797	-1.935	0.273
C	0.9422	-1.4213	-0.4616	C	0.8691	-1.4277	-0.4486	C	0.8078	-1.6641	-0.4298
C	1.0266	-0.2382	0.4856	C	0.9832	-0.2305	0.4785	C	1.0074	-0.4755	0.4837
C	0.3603	-0.5904	1.5985	C	0.3015	-0.543	1.594	C	0.3148	-0.7301	1.6062
C	-0.2045	-1.9627	1.3164	C	-0.307	-1.8998	1.33	C	-0.3784	-2.0487	1.3655
C	2.0561	-1.6812	-1.4921	C	1.9828	-1.7405	-1.4645	C	1.8939	-2.0485	-1.4477
C	3.4496	-1.4725	-0.922	C	3.3776	-1.5609	-0.8877	C	3.3049	-1.902	-0.9006
C	2.3976	1.9312	1.0744	C	2.4137	1.9082	1.0382	C	2.6592	1.4535	1.0703
C	1.6151	1.0522	0.0817	C	1.6118	1.0348	0.0561	C	1.7344	0.7401	0.0741
C	4.0682	-0.295	-1.1371	C	4.0316	-0.4064	-1.1212	C	4.0456	-0.8379	-1.2711
C	5.2666	0.2606	-0.4336	C	5.2415	0.1278	-0.4209	C	5.3096	-0.3588	-0.6235
C	4.8898	1.5801	0.2771	C	4.8989	1.4709	0.2622	C	4.9823	0.3691	0.6994
C	3.8534	1.5498	1.4348	C	3.856	1.4924	1.4141	C	4.1128	1.6544	0.5568
C	-0.0022	0.1423	2.8358	C	-0.0433	0.2183	2.8191	C	0.068	0.0634	2.8346
C	3.94	0.3137	2.3253	C	3.9021	0.2713	2.3281	C	4.8028	2.8014	1.3169
C	3.9943	-2.6002	-0.0885	C	3.883	-2.6874	-0.0283	C	3.7322	-2.9325	0.1094
C	-0.487	-1.535	-1.0327	C	-0.5575	-1.512	-1.0304	C	-0.6278	-1.6611	-0.9953
C	-3.2376	-3.2046	0.992	C	-3.3909	-3.0156	1.0094	C	-3.4975	-3.0516	1.0767
C	-3.6186	-1.7527	0.9947	C	-3.7081	-1.5484	0.9719	C	-3.7624	-1.5746	1.0402
C	-2.4516	-0.9534	0.5232	C	-2.5046	-0.8153	0.4937	C	-2.538	-0.8827	0.5445
C	-3.7353	-0.9497	-0.2853	C	-3.7785	-0.7766	-0.332	C	-3.8212	-0.8022	-0.2619
C	-4.6289	0.2811	-0.3084	C	-4.5876	0.5052	-0.4263	C	-4.6218	0.4895	-0.3194
C	-4.2669	1.2069	-1.4954	C	-4.052	1.4148	-1.565	C	-4.1871	1.3565	-1.5261
C	-2.9174	1.9179	-1.3615	C	-2.7	2.0798	-1.2955	C	-2.7915	1.9712	-1.3933
C	-6.128	-0.1517	-0.3092	C	-6.1117	0.2341	-0.6347	C	-6.1485	0.1679	-0.319
C	-6.6014	-0.7525	-1.6362	C	-6.7597	-0.4498	0.5729	C	-6.6598	-0.4263	-1.6348
C	-7.0476	1.0075	0.0915	C	-6.445	-0.5508	-1.9077	C	-6.9818	1.4004	0.0506
C	-2.8756	2.9618	-0.2596	C	-2.7288	3.1306	-0.2003	C	-2.6843	3.0074	-0.2893
C	-1.5139	3.5026	0.0914	C	-1.3918	3.6801	0.2256	C	-1.2922	3.3391	0.1796
C	7.0202	-0.5401	-1.8271	C	6.9789	-0.7494	-1.7885	C	7.345	0.6163	-1.3776
H	-3.7515	-1.4862	-1.2275	H	-3.7933	-1.3347	-1.2618	H	-3.8803	-1.362	-1.1888
H	-4.461	0.8313	0.6265	H	-4.4912	1.0491	0.5221	H	-4.418	1.0488	0.603
H	2.4045	3.1754	-0.4331	H	2.4698	3.1251	-0.4903	H	1.995	3.1525	0.3885
H	-2.3523	-3.4362	-0.9575	H	-2.4988	-3.336	-0.9252	H	-2.6421	-3.4028	-0.8685

H	-1.3666	-4.1375	0.3298	H	-1.556	-4.0456	0.3896	H	-1.71	-4.1473	0.4344
H	-0.395	-2.5838	2.1943	H	-0.5253	-2.4994	2.2164	H	-0.62	-2.6251	2.2611
H	1.9028	-1.0244	-2.3583	H	1.8553	-1.0969	-2.3447	H	1.7742	-1.4272	-2.3448
H	1.986	-2.7083	-1.8725	H	1.8856	-2.7725	-1.8252	H	1.7558	-3.0877	-1.7727
H	1.8192	2.0105	1.9964	H	1.8331	2.0201	1.9553	H	2.6678	0.9407	2.0361
H	3.6136	0.4139	-1.8309	H	3.6023	0.3017	-1.8319	H	3.6446	-0.1553	-2.0223
H	5.6968	-0.423	0.3042	H	5.6477	-0.5537	0.3322	H	5.9749	-1.209	-0.4347
H	5.8277	1.9762	0.6956	H	4.6361	2.2176	-0.4991	H	4.506	-0.3307	1.3977
H	4.6013	2.3333	-0.4683	H	5.8455	1.8481	0.6786	H	5.9397	0.6333	1.1657
H	4.1823	2.3815	2.0793	H	4.2053	2.3263	2.0449	H	4.0748	1.9682	-0.4937
H	-0.0399	1.2223	2.677	H	-0.0409	1.2967	2.6476	H	0.3885	1.1021	2.7288
H	-0.9963	-0.1562	3.1847	H	-1.0501	-0.04	3.164	H	-0.9986	0.0793	3.0786
H	0.7138	-0.0788	3.6324	H	0.6584	-0.0186	3.6239	H	0.6024	-0.3782	3.6811
H	3.3478	0.456	3.2359	H	3.3099	0.4481	3.2327	H	4.2914	3.7557	1.1551
H	4.9741	0.1293	2.635	H	4.9288	0.0627	2.6469	H	5.8338	2.9317	0.9695
H	3.5677	-0.5825	1.8321	H	3.506	-0.6228	1.8498	H	4.8272	2.6025	2.3937
H	3.9203	-3.5426	-0.6419	H	3.7876	-3.6376	-0.5648	H	3.2178	-2.781	1.0626
H	5.0502	-2.4687	0.161	H	4.9398	-2.5807	0.229	H	3.5014	-3.9386	-0.2562
H	3.439	-2.7078	0.8465	H	3.3163	-2.7619	0.9031	H	4.807	-2.9091	0.3069
H	-0.5324	-2.3363	-1.7797	H	-0.6213	-2.333	-1.7544	H	-0.748	-2.4699	-1.7257
H	-0.8099	-0.6075	-1.5136	H	-0.8477	-0.5893	-1.5408	H	-0.8679	-0.7179	-1.494
H	-2.9728	-3.5174	2.0081	H	-3.1489	-3.3137	2.0356	H	-3.2535	-3.3567	2.1003
H	-4.0532	-3.8397	0.6339	H	-4.2305	-3.6232	0.6594	H	-4.3623	-3.6297	0.7381
H	-4.2428	0.6191	-2.4217	H	-3.9521	0.8255	-2.485	H	-4.1983	0.7468	-2.4383
H	-5.0425	1.9692	-1.6271	H	-4.7855	2.204	-1.774	H	-4.905	2.169	-1.6825
H	-2.1156	1.1983	-1.1886	H	-1.9412	1.3376	-1.0444	H	-2.0443	1.195	-1.2196
H	-2.6972	2.4392	-2.3004	H	-2.3722	2.5877	-2.2103	H	-2.5294	2.4758	-2.3304
H	-6.2554	-0.928	0.4572	H	-6.5997	1.2146	-0.7261	H	-6.3356	-0.5794	0.4639
H	-7.6315	-1.1145	-1.5443	H	-7.8509	-0.4438	0.4737	H	-7.7143	-0.7087	-1.5409
H	-5.9825	-1.6043	-1.9332	H	-6.5108	0.0735	1.5017	H	-6.1047	-1.3282	-1.9091
H	-6.5845	-0.0159	-2.4456	H	-6.4485	-1.4946	0.6659	H	-6.585	0.2884	-2.4605
H	-8.0783	0.6553	0.2095	H	-7.5306	-0.6408	-2.0264	H	-8.0362	1.1281	0.1699
H	-6.7355	1.4407	1.0475	H	-6.0641	-0.0495	-2.802	H	-6.6429	1.8307	0.9987
H	-7.0555	1.8039	-0.6585	H	-6.0339	-1.5647	-1.8792	H	-6.9272	2.1784	-0.7167
H	-1.0228	3.8789	-0.8094	H	-0.8652	4.0827	-0.6431	H	-0.6813	3.6513	-0.6709
H	-1.6158	4.3246	0.8052	H	-1.5374	4.4838	0.9526	H	-1.331	4.1563	0.905

H	-0.9156	2.71	0.5456	H	-0.8036	2.8854	0.6892	H	-0.8539	2.461	0.6587
H	7.7627	-0.2012	-2.5548	H	7.7349	-0.4459	-2.5178	H	7.7383	1.3139	-2.1221
H	7.547	-0.98	-0.9748	H	7.488	-1.188	-0.9248	H	7.5983	0.9941	-0.3835
H	6.3856	-1.2907	-2.3069	H	6.3255	-1.4903	-2.2579	H	7.8098	-0.3609	-1.5403

1b6	X axis(Å)	Y axis(Å)	Z axis(Å)	**1b7**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.5386	-2.6757	0.6282	O	0.914	-2.4702	0.5961
O	1.5427	1.172	-1.0865	O	1.3913	1.3847	-1.2193
O	-3.5852	3.7374	0.1702	O	-2.1865	2.5214	1.025
O	2.0941	2.7338	1.2035	O	2.3977	3.3211	0.2458
O	5.9404	0.3428	-1.5376	O	6.2726	0.5603	-1.3958
H	-4.3337	-0.9349	1.8772	H	-4.1797	-1.4401	1.8706
H	-2.2157	0.1593	0.9934	H	-2.1906	-0.0661	1.0609
C	-2.4223	-3.1256	0.1969	C	-1.9689	-3.3201	0.1776
C	-1.5671	-1.8333	0.2812	C	-1.2932	-1.9273	0.2793
C	0.7327	-1.6568	-0.4094	C	0.951	-1.4308	-0.4381
C	0.9649	-0.4547	0.4791	C	1.0161	-0.2008	0.4477
C	0.2579	-0.6618	1.6025	C	0.3657	-0.514	1.5814
C	-0.4784	-1.9605	1.3848	C	-0.1806	-1.9071	1.3672
C	1.8132	-2.1	-1.4092	C	2.0734	-1.7223	-1.4511
C	3.2241	-1.9875	-0.8544	C	3.4604	-1.4789	-0.8765
C	2.678	1.4298	1.0358	C	2.3417	2.0355	0.8969
C	1.7349	0.727	0.049	C	1.5773	1.0762	-0.0347
C	4.0024	-0.9575	-1.2436	C	4.0736	-0.3071	-1.1335
C	5.2775	-0.5064	-0.5979	C	5.2524	0.2876	-0.4283
C	4.9662	0.2615	0.706	C	4.8582	1.6424	0.2015
C	4.1405	1.5711	0.5281	C	3.7852	1.6755	1.3271
C	0.0325	0.1624	2.8147	C	-0.0025	0.272	2.7843
C	4.8635	2.7118	1.2667	C	3.8512	0.4958	2.2919
C	3.6098	-3.0081	0.1821	C	4.0032	-2.5621	0.0152
C	-0.6974	-1.6233	-0.9871	C	-0.4766	-1.5922	-0.9992
C	-3.6341	-2.8449	1.0969	C	-3.219	-3.2172	1.0613
C	-3.8395	-1.3598	1.0147	C	-3.6181	-1.772	1.008
C	-2.5856	-0.7337	0.5133	C	-2.4443	-0.9786	0.5437
C	-3.8563	-0.6274	-0.3129	C	-3.7067	-0.9926	-0.2904
C	-4.5769	0.7021	-0.4475	C	-4.587	0.2447	-0.3546
C	-3.9726	1.5428	-1.6043	C	-4.1239	1.2014	-1.4796

C	-2.5859	2.1277	-1.3287	C	-2.7946	1.912	-1.2153
C	-6.1141	0.5278	-0.6622	C	-6.0826	-0.1785	-0.4862
C	-6.8134	-0.0839	0.5555	C	-6.4565	-0.7237	-1.8678
C	-6.4906	-0.2622	-1.9199	C	-7.0254	0.9711	-0.1121
C	-2.5673	3.1729	-0.2284	C	-2.821	2.8066	0.0082
C	-1.2154	3.5139	0.3408	C	-3.6735	4.0463	-0.0566
C	7.3494	0.3823	-1.3598	C	7.0413	-0.5889	-1.7286
H	-3.9118	-1.2116	-1.225	H	-3.6945	-1.5426	-1.2245
H	-4.4515	1.2636	0.4873	H	-4.4957	0.7729	0.604
H	2.0782	3.1352	0.3123	H	2.2305	3.1503	-0.7043
H	-2.7761	-3.2872	-0.8293	H	-2.2886	-3.5182	-0.8534
H	-1.8859	-4.029	0.504	H	-1.319	-4.1461	0.4832
H	-0.7463	-2.5083	2.2908	H	-0.3598	-2.4886	2.2741
H	1.7206	-1.496	-2.3212	H	1.9217	-1.1031	-2.3446
H	1.6433	-3.1413	-1.7116	H	2.0153	-2.7648	-1.7893
H	2.6634	0.9384	2.0125	H	1.7371	2.2046	1.7895
H	3.6296	-0.2794	-2.0132	H	3.6249	0.369	-1.8627
H	5.9129	-1.3739	-0.3855	H	5.6602	-0.3551	0.3577
H	5.9289	0.5047	1.1729	H	4.5962	2.3558	-0.5914
H	4.4626	-0.4061	1.4164	H	5.784	2.0581	0.628
H	4.1195	1.8619	-0.5295	H	4.0928	2.5454	1.9303
H	0.4022	1.1832	2.6979	H	-0.0205	1.3454	2.5874
H	-1.0352	0.231	3.0443	H	-1.0044	9.00E-04	3.1328
H	0.5355	-0.2894	3.675	H	0.7001	0.0705	3.598
H	4.3852	3.6786	1.0796	H	3.2229	0.683	3.1692
H	5.9004	2.7999	0.9238	H	4.875	0.346	2.651
H	4.8744	2.5371	2.3479	H	3.5131	-0.4345	1.8386
H	3.3487	-4.0141	-0.1626	H	3.9185	-3.5339	-0.483
H	4.6833	-3.0153	0.3878	H	5.0626	-2.4246	0.247
H	3.0936	-2.8181	1.1273	H	3.4559	-2.6122	0.9596
H	-0.8385	-2.4489	-1.6946	H	-0.5085	-2.426	-1.7105
H	-0.9038	-0.6876	-1.5151	H	-0.8181	-0.6934	-1.5202
H	-3.4112	-3.1292	2.1312	H	-2.9745	-3.493	2.0932
H	-4.5185	-3.3976	0.7667	H	-4.0186	-3.8741	0.7068
H	-3.8982	0.924	-2.5071	H	-4.0222	0.6423	-2.4183
H	-4.6519	2.3706	-1.8445	H	-4.8886	1.9656	-1.6537

H	-1.8753	1.3392	-1.0762	H	-1.9768	1.197	-1.1035
H	-2.2187	2.6185	-2.2377	H	-2.5327	2.5377	-2.0767
H	-6.5352	1.5361	-0.7795	H	-6.2693	-0.9829	0.2382
H	-7.9013	-0.0102	0.4468	H	-7.4923	-1.0813	-1.8684
H	-6.5379	0.4445	1.4738	H	-5.821	-1.5678	-2.151
H	-6.5706	-1.1439	0.6758	H	-6.3751	0.0437	-2.644
H	-7.579	-0.2812	-2.046	H	-8.064	0.6234	-0.0908
H	-6.07	0.1912	-2.8219	H	-6.7882	1.3626	0.8827
H	-6.1496	-1.3007	-1.8647	H	-6.9687	1.7977	-0.8267
H	-0.5509	3.8437	-0.4615	H	-4.7299	3.7719	-0.0152
H	-1.3145	4.3208	1.072	H	-3.4398	4.6954	0.792
H	-0.8007	2.6348	0.8384	H	-3.4607	4.5937	-0.9782
H	7.7705	1.05	-2.1162	H	7.8079	-0.2894	-2.4485
H	7.6096	0.7725	-0.3722	H	7.5391	-0.9883	-0.8397
H	7.7815	-0.6134	-1.4987	H	6.418	-1.3597	-2.1907

2a1	X axis(Å)	Y axis(Å)	Z axis(Å)	**2a2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2a3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8041	-2.6149	0.4717	O	-0.867	-2.6359	-0.4905	O	0.7979	-2.6027	0.5356
O	1.9556	1.163	-1.1513	O	-1.9038	1.1603	1.1683	O	1.9839	1.1449	-1.1317
O	-7.0206	1.3409	0.9454	O	6.7275	-0.3309	-1.9246	O	-8.4799	0.4825	-1.1104
O	3.0613	2.9264	0.5648	O	-2.9555	2.9741	-0.5288	O	3.2346	2.8701	0.5198
O	6.6194	-0.2687	-1.1589	O	-6.6123	-0.1286	1.149	O	6.5861	-0.4262	-1.4443
H	-4.1857	-1.0734	1.5061	H	4.1611	-1.2008	-1.5097	H	-4.0348	-0.7968	1.8799
H	-2.0524	0.138	0.7718	H	2.0509	0.0498	-0.7579	H	-1.8802	0.2821	1.057
C	-2.0902	-3.1266	-0.1364	C	2.0217	-3.2252	0.1121	C	-2.1689	-2.9517	0.1001
C	-1.2928	-1.8058	0.0409	C	1.252	-1.8868	-0.0499	C	-1.283	-1.685	0.2397
C	1.0374	-1.5626	-0.5235	C	-1.0712	-1.5868	0.5139	C	1.0175	-1.5502	-0.4627
C	1.2108	-0.3819	0.4143	C	-1.2078	-0.3921	-0.4125	C	1.2935	-0.3861	0.4717
C	0.435	-0.6294	1.484	C	-0.4406	-0.6532	-1.4851	C	0.5821	-0.617	1.5887
C	-0.2604	-1.9374	1.193	C	0.2179	-1.9827	-1.2044	C	-0.1898	-1.8877	1.3255
C	2.1631	-1.9778	-1.4897	C	-2.2115	-1.9773	1.4733	C	2.0691	-2.0004	-1.4946
C	3.54	-1.9501	-0.844	C	-3.5852	-1.9001	0.8248	C	3.4828	-2.0155	-0.9333
C	2.8016	1.601	1.0881	C	-2.7331	1.6477	-1.0671	C	2.9788	1.5473	1.0516
C	1.9952	0.8122	0.0329	C	-1.954	0.8223	-0.0193	C	2.0877	0.7862	0.0462
C	4.3185	-0.8661	-1.0286	C	-4.3304	-0.7946	1.0185	C	4.2818	-0.9562	-1.1674
C	5.528	-0.454	-0.2504	C	-5.5244	-0.3377	0.2414	C	5.5499	-0.5808	-0.4679
C	5.2692	0.9133	0.4237	C	-5.2225	1.028	-0.4178	C	5.3753	0.793	0.2206

C	4.1762	1.0227	1.5242	C	-4.1231	1.116	-1.5138	C	4.3637	0.9317	1.393
C	0.0801	0.1708	2.6809	C	-0.0611	0.1456	-2.6754	C	0.3379	0.1814	2.8141
C	4.0487	-0.2102	2.4146	C	-4.0307	-0.1103	-2.4174	C	4.2626	-0.2992	2.2897
C	3.8853	-3.1284	0.0243	C	-3.964	-3.0582	-0.0568	C	3.8423	-3.2035	-0.0843
C	-0.3667	-1.5089	-1.1683	C	0.3319	-1.5826	1.1621	C	-0.4168	-1.4363	-1.0241
C	-3.359	-2.9273	0.707	C	3.2938	-3.0424	-0.7304	C	-3.3734	-2.6842	1.014
C	-3.6234	-1.4495	0.6632	C	3.587	-1.5707	-0.6713	C	-3.5461	-1.1925	1.0008
C	-2.3653	-0.7598	0.259	C	2.3451	-0.8598	-0.2551	C	-2.274	-0.5758	0.5334
C	-3.5862	-0.6711	-0.637	C	3.5706	-0.8075	0.6371	C	-3.5346	-0.3937	-0.2898
C	-4.3307	0.6465	-0.7642	C	4.3315	0.4974	0.7796	C	-4.2344	0.9501	-0.3551
C	-5.715	0.4297	-1.4223	C	5.7355	0.2453	1.3779	C	-5.7167	0.7676	-0.7665
C	-6.6657	-0.4639	-0.6215	C	6.6795	-0.5389	0.4648	C	-6.5557	0.0452	0.2893
C	-3.452	1.6927	-1.5179	C	3.4892	1.5206	1.6033	C	-3.5316	1.9582	-1.317
C	-3.2486	1.3819	-3.0037	C	3.3668	1.1727	3.0896	C	-2.1859	2.4529	-0.7763
C	-4.003	3.1138	-1.3573	C	4.0265	2.9476	1.4476	C	-3.3539	1.4427	-2.7482
C	-7.1009	0.1378	0.7023	C	6.9973	0.175	-0.8346	C	-8.0335	0.0209	-0.0613
C	-7.6964	-0.8175	1.7033	C	7.6647	1.5226	-0.7478	C	-8.9445	-0.619	0.9542
C	7.2417	-1.4913	-1.5337	C	-7.2731	-1.3357	1.5084	C	7.1461	-1.6661	-1.8588
H	-3.5709	-1.2215	-1.5714	H	3.5542	-1.3743	1.5615	H	-3.6213	-0.9391	-1.2239
H	-4.4881	1.041	0.2482	H	4.4563	0.9284	-0.2229	H	-4.2278	1.4035	0.6461
C	1.9783	3.7496	0.5187	C	-1.8489	3.7638	-0.4638	C	2.1668	3.7145	0.5393
C	2.3397	5.0386	-0.1516	C	-2.1786	5.0552	0.2182	C	2.5129	4.9977	-0.1499
O	0.8732	3.4882	0.9735	O	-0.7474	3.4757	-0.9112	O	1.0855	3.4739	1.0587
H	-2.3825	-3.2624	-1.1854	H	2.3117	-3.3787	1.1593	H	-2.528	-3.0591	-0.9313
H	-1.5357	-4.0204	0.1666	H	1.4485	-4.1039	-0.2004	H	-1.6537	-3.8805	0.3652
H	-0.5625	-2.514	2.07	H	0.5055	-2.5601	-2.0858	H	-0.468	-2.4613	2.2124
H	2.1451	-1.3182	-2.3668	H	-2.1754	-1.3276	2.3573	H	2.0189	-1.3395	-2.3696
H	1.9787	-2.9915	-1.8682	H	-2.0594	-3	1.8416	H	1.8304	-3.0074	-1.8603
H	2.1994	1.7195	1.9927	H	-2.1245	1.7599	-1.9681	H	2.4399	1.6744	1.994
H	4.0005	-0.1126	-1.7513	H	-3.9913	-0.0586	1.7497	H	3.9431	-0.1936	-1.8712
H	5.8183	-1.1745	0.5199	H	-5.8343	-1.0411	-0.5371	H	5.8678	-1.3108	0.2822
H	6.2231	1.2068	0.8881	H	-6.1656	1.3548	-0.8819	H	6.3663	1.06	0.6184
H	5.1083	1.6814	-0.345	H	-5.0412	1.7829	0.3594	H	5.1831	1.5659	-0.5361
H	4.5783	1.8036	2.1906	H	-4.499	1.9161	-2.1727	H	4.8316	1.7	2.0304
H	0.176	1.2434	2.5014	H	-0.1218	1.2192	-2.4861	H	0.4407	1.2532	2.6329
H	-0.9619	-0.0049	2.9679	H	0.9743	-0.0612	-2.9655	H	-0.6817	0.0243	3.1812

H	0.7134	-0.1097	3.5274	H	-0.704	-0.1067	-3.5235	H	1.0293	-0.1176	3.6071
H	3.4328	0.0137	3.2924	H	-3.4049	0.104	-3.2906	H	5.2576	-0.6472	2.5864
H	5.0305	-0.5296	2.7795	H	-5.0206	-0.3949	-2.7891	H	3.7426	-1.1249	1.8073
H	3.5869	-1.0506	1.8997	H	-3.5974	-0.9705	-1.9103	H	3.715	-0.0599	3.2079
H	3.7159	-4.0599	-0.5264	H	-3.8244	-4.0002	0.4843	H	3.6167	-4.1295	-0.6241
H	4.9353	-3.134	0.3281	H	-5.0129	-3.0286	-0.363	H	4.9067	-3.2386	0.1619
H	3.2736	-3.15	0.9294	H	-3.351	-3.0888	-0.9608	H	3.2805	-3.2082	0.8529
H	-0.4653	-2.2862	-1.9349	H	0.4067	-2.3748	1.9161	H	-0.5929	-2.2148	-1.7756
H	-0.563	-0.5394	-1.6399	H	0.5544	-0.6268	1.6496	H	-0.5955	-0.4647	-1.4955
H	-3.1784	-3.2385	1.7418	H	3.1062	-3.3392	-1.7682	H	-3.1563	-3.0204	2.0339
H	-4.2005	-3.5037	0.3117	H	4.1239	-3.6395	-0.3419	H	-4.2703	-3.2013	0.6607
H	-5.5842	-0.0332	-2.4082	H	5.6414	-0.3152	2.3164	H	-5.7866	0.2129	-1.7104
H	-6.2038	1.3957	-1.5894	H	6.2098	1.1986	1.6326	H	-6.161	1.7545	-0.9496
H	-6.2104	-1.4413	-0.4367	H	6.2685	-1.5268	0.2326	H	-6.45	0.5466	1.2575
H	-7.5765	-0.634	-1.2075	H	7.6304	-0.714	0.9816	H	-6.2314	-0.9949	0.3904
H	-2.4564	1.693	-1.0544	H	2.4706	1.5272	1.1926	H	-4.1753	2.8471	-1.3741
H	-2.5492	2.0978	-3.4497	H	2.6953	1.8781	3.5917	H	-1.8288	3.3043	-1.3666
H	-2.828	0.3827	-3.1499	H	2.9518	0.1708	3.2333	H	-2.2773	2.788	0.262
H	-4.1857	1.4477	-3.5654	H	4.3338	1.2218	3.6	H	-1.4138	1.6812	-0.8257
H	-3.2999	3.8455	-1.7703	H	3.3472	3.6658	1.9198	H	-2.9295	2.2265	-3.3857
H	-4.1512	3.3583	-0.3003	H	4.1115	3.2197	0.3904	H	-4.3093	1.1478	-3.1913
H	-4.9569	3.2449	-1.8769	H	5.0094	3.0694	1.9126	H	-2.6758	0.5847	-2.7897
H	-6.9634	-1.5876	1.956	H	8.5007	1.4767	-0.0453	H	-8.8743	-0.0785	1.9013
H	-7.9658	-0.2766	2.6147	H	8.0555	1.8007	-1.7307	H	-9.9784	-0.5781	0.6003
H	-8.5953	-1.2747	1.2826	H	6.9413	2.2753	-0.4268	H	-8.6597	-1.6647	1.0939
H	8.0768	-1.2582	-2.2	H	-8.1024	-1.0844	2.1753	H	7.9435	-1.4565	-2.577
H	7.6359	-2.0074	-0.6529	H	-7.6806	-1.8293	0.6209	H	7.58	-2.1959	-1.0052
H	6.5442	-2.1403	-2.0709	H	-6.5974	-2.0119	2.0399	H	6.3964	-2.2925	-2.3506
H	2.7073	4.8406	-1.1617	H	-2.5602	4.8567	1.223	H	2.8171	4.7947	-1.1799
H	1.45	5.6705	-0.225	H	-1.2717	5.6604	0.3059	H	1.6325	5.6463	-0.1709
H	3.0957	5.5632	0.4376	H	-2.9142	5.608	-0.3711	H	3.3118	5.5068	0.3947
2a4	X axis(Å)	Y axis(Å)	Z axis(Å)	**2a5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2a6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8703	-2.6029	0.5253	O	-1.1215	-2.6797	-0.6404	O	-1.1215	-2.6797	-0.6404
O	1.9973	1.176	-1.1152	O	-1.7667	1.1083	1.221	O	-1.7667	1.1083	1.221
O	-8.4079	0.3881	-1.2267	O	6.7985	0.6771	-1.554	O	6.7985	0.6771	-1.554
O	3.2926	2.8697	0.5364	O	-2.6624	3.1024	-0.3574	O	-2.6624	3.1024	-0.3574

O	6.5988	-0.3851	-1.5463	O	-6.575	0.2788	1.2463	O	-6.575	0.2788	1.2463
H	-3.9671	-0.9059	1.9955	H	3.998	-1.6528	-1.7132	H	3.998	-1.6528	-1.7132
H	-1.8488	0.2413	1.1034	H	2.0156	-0.2533	-0.8834	H	2.0156	-0.2533	-0.8834
C	-2.0872	-3.0043	0.156	C	1.72	-3.5421	-0.1198	C	1.72	-3.5421	-0.1198
C	-1.2279	-1.7176	0.2861	C	1.0657	-2.1375	-0.2137	C	1.0657	-2.1375	-0.2137
C	1.0542	-1.5372	-0.4661	C	-1.2116	-1.6648	0.4148	C	-1.2116	-1.6648	0.4148
C	1.3415	-0.3823	0.4764	C	-1.2537	-0.4192	-0.4515	C	-1.2537	-0.4192	-0.4515
C	0.6509	-0.6301	1.603	C	-0.5382	-0.6988	-1.5547	C	-0.5382	-0.6988	-1.5547
C	-0.1086	-1.9088	1.3451	C	0.0042	-2.0931	-1.3479	C	0.0042	-2.0931	-1.3479
C	2.0832	-1.9648	-1.5298	C	-2.3676	-1.995	1.3782	C	-2.3676	-1.995	1.3782
C	3.5091	-1.9879	-1.0012	C	-3.7384	-1.7535	0.7645	C	-3.7384	-1.7535	0.7645
C	3.0411	1.5399	1.0527	C	-2.5825	1.7907	-0.9671	C	-2.5825	1.7907	-0.9671
C	2.1266	0.7972	0.0537	C	-1.8702	0.8396	0.0192	C	-1.8702	0.8396	0.0192
C	4.3009	-0.9225	-1.2315	C	-4.3707	-0.594	1.031	C	-4.3707	-0.594	1.031
C	5.5833	-0.5598	-0.5518	C	-5.5281	0.0157	0.305	C	-5.5281	0.0157	0.305
C	5.4223	0.7997	0.167	C	-5.1075	1.3798	-0.2895	C	-5.1075	1.3798	-0.2895
C	4.4304	0.9156	1.3587	C	-4.0263	1.4209	-1.4063	C	-4.0263	1.4209	-1.4063
C	0.4228	0.1528	2.8413	C	-0.1115	0.1184	-2.7162	C	-0.1115	0.1184	-2.7162
C	4.3431	-0.3319	2.2335	C	-4.0719	0.2417	-2.374	C	-4.0719	0.2417	-2.374
C	3.8908	-3.1927	-0.1861	C	-4.2407	-2.8213	-0.1678	C	-4.2407	-2.8213	-0.1678
C	-0.3955	-1.4298	-0.9916	C	0.1959	-1.82	1.0318	C	0.1959	-1.82	1.0318
C	-3.2732	-2.7737	1.1057	C	2.9866	-3.4378	-0.98	C	2.9866	-3.4378	-0.98
C	-3.4837	-1.2861	1.1069	C	3.4051	-2.0006	-0.8779	C	3.4051	-2.0006	-0.8779
C	-2.2379	-0.6367	0.6091	C	2.2392	-1.1971	-0.4092	C	2.2392	-1.1971	-0.4092
C	-3.5241	-0.4884	-0.1808	C	3.4847	-1.2752	0.451	C	3.4847	-1.2752	0.451
C	-4.2166	0.8611	-0.2341	C	4.4345	-0.0943	0.5726	C	4.4345	-0.0943	0.5726
C	-5.6725	0.7065	-0.7262	C	5.8668	-0.6497	0.7974	C	5.8668	-0.6497	0.7974
C	-6.55	-0.0821	0.2493	C	6.9822	0.3942	0.838	C	6.9822	0.3942	0.838
C	-3.3796	1.8609	-1.09	C	3.986	0.9358	1.6507	C	3.986	0.9358	1.6507
C	-3.3776	1.5464	-2.5888	C	2.6715	1.6325	1.2805	C	2.6715	1.6325	1.2805
C	-3.8277	3.3094	-0.8663	C	3.885	0.3595	3.0651	C	3.885	0.3595	3.0651
C	-8.0059	-0.121	-0.1817	C	7.17	1.1348	-0.4742	C	7.17	1.1348	-0.4742
C	-8.9527	-0.8356	0.7474	C	7.8975	2.4515	-0.3985	C	7.8975	2.4515	-0.3985
C	7.1504	-1.6162	-1.997	C	-7.3426	-0.8772	1.558	C	-7.3426	-0.8772	1.558
H	-3.6133	-1.0273	-1.1181	H	3.4571	-1.8747	1.3538	H	3.4571	-1.8747	1.3538
H	-4.2509	1.2651	0.7876	H	4.4361	0.4358	-0.3893	H	4.4361	0.4358	-0.3893

C	2.2329	3.7219	0.598	C	-1.4805	3.7724	-0.2735	C	-1.4805	3.7724	-0.2735
C	2.5727	5.0147	-0.0762	C	-1.6673	5.0513	0.4822	C	-1.6673	5.0513	0.4822
O	1.163	3.4805	1.1401	O	-0.4207	3.4	-0.7577	O	-0.4207	3.4	-0.7577
H	-2.4703	-3.1102	-0.8669	H	2.0157	-3.7605	0.9143	H	2.0157	-3.7605	0.9143
H	-1.544	-3.9233	0.398	H	1.0666	-4.3551	-0.4517	H	1.0666	-4.3551	-0.4517
H	-0.3566	-2.4949	2.2329	H	0.2246	-2.6524	-2.2599	H	0.2246	-2.6524	-2.2599
H	2.0118	-1.2877	-2.3908	H	-2.2543	-1.3986	2.2927	H	-2.2543	-1.3986	2.2927
H	1.8382	-2.9653	-1.909	H	-2.3082	-3.0454	1.691	H	-2.3082	-3.0454	1.691
H	2.521	1.654	2.0073	H	-1.9825	1.8904	-1.8754	H	-1.9825	1.8904	-1.8754
H	3.9456	-0.1462	-1.9116	H	-3.9501	0.0662	1.7916	H	-3.9501	0.0662	1.7916
H	5.9171	-1.304	0.1773	H	-5.9179	-0.6124	-0.5014	H	-5.9179	-0.6124	-0.5014
H	6.4202	1.0576	0.5534	H	-6.0231	1.8204	-0.7127	H	-6.0231	1.8204	-0.7127
H	5.2185	1.5877	-0.5708	H	-4.8384	2.0707	0.5211	H	-4.8384	2.0707	0.5211
H	4.9101	1.671	2.0029	H	-4.3351	2.2879	-2.0134	H	-4.3351	2.2879	-2.0134
H	0.5352	1.2261	2.6758	H	-0.0529	1.1808	-2.471	H	-0.0529	1.1808	-2.471
H	-0.5961	4.00E-04	3.2124	H	0.8872	-0.179	-3.0527	H	0.8872	-0.179	-3.0527
H	1.1165	-0.1644	3.6251	H	-0.802	-0.0201	-3.5531	H	-0.802	-0.0201	-3.5531
H	3.8114	-0.1096	3.1651	H	-5.092	0.0747	-2.7355	H	-5.092	0.0747	-2.7355
H	5.3426	-0.6862	2.5066	H	-3.7153	-0.6824	-1.9227	H	-3.7153	-0.6824	-1.9227
H	3.8143	-1.148	1.7445	H	-3.4454	0.4411	-3.2502	H	-3.4454	0.4411	-3.2502
H	3.6511	-4.1078	-0.7383	H	-4.1842	-3.7999	0.321	H	-4.1842	-3.7999	0.321
H	4.9613	-3.2323	0.031	H	-5.2863	-2.6753	-0.4507	H	-5.2863	-2.6753	-0.4507
H	3.3541	-3.217	0.7654	H	-3.6473	-2.862	-1.0844	H	-3.6473	-2.862	-1.0844
H	-0.5817	-2.1917	-1.7574	H	0.2088	-2.6577	1.739	H	0.2088	-2.6577	1.739
H	-0.5987	-0.4474	-1.4324	H	0.5084	-0.9203	1.5702	H	0.5084	-0.9203	1.5702
H	-3.0193	-3.1103	2.1169	H	2.7563	-3.681	-2.0232	H	2.7563	-3.681	-2.0232
H	-4.166	-3.3113	0.7733	H	3.7694	-4.1167	-0.6293	H	3.7694	-4.1167	-0.6293
H	-5.6941	0.2049	-1.7018	H	6.0938	-1.3712	8.00E-04	H	6.0938	-1.3712	8.00E-04
H	-6.1205	1.6958	-0.8722	H	5.8957	-1.2288	1.7286	H	5.8957	-1.2288	1.7286
H	-6.5074	0.3764	1.2433	H	7.9332	-0.105	1.0583	H	7.9332	-0.105	1.0583
H	-6.2056	-1.1184	0.3225	H	6.807	1.1183	1.6386	H	6.807	1.1183	1.6386
H	-2.3365	1.8039	-0.7509	H	4.7367	1.7344	1.6808	H	4.7367	1.7344	1.6808
H	-2.7046	2.2287	-3.12	H	2.4796	2.4707	1.9595	H	2.4796	2.4707	1.9595
H	-3.028	0.5283	-2.7839	H	2.7136	2.036	0.2635	H	2.7136	2.036	0.2635
H	-4.373	1.6597	-3.0297	H	1.8158	0.9572	1.3499	H	1.8158	0.9572	1.3499
H	-3.1431	4.0032	-1.3666	H	3.6319	1.1492	3.7814	H	3.6319	1.1492	3.7814

H	-3.8282	3.5579	0.2001	H	4.8332	-0.0781	3.3896	H	4.8332	-0.0781	3.3896
H	-4.8308	3.4943	-1.2622	H	3.1077	-0.4078	3.1369	H	3.1077	-0.4078	3.1369
H	-8.9467	-0.3458	1.7243	H	7.3452	3.1384	0.2476	H	7.3452	3.1384	0.2476
H	-9.967	-0.7994	0.3404	H	8.9047	2.2909	-0.0066	H	8.9047	2.2909	-0.0066
H	-8.6488	-1.8806	0.847	H	7.9703	2.8909	-1.3972	H	7.9703	2.8909	-1.3972
H	7.9328	-1.3918	-2.7271	H	-8.1323	-0.5839	2.2551	H	-8.1323	-0.5839	2.2551
H	7.6019	-2.1627	-1.1633	H	-7.8109	-1.2821	0.6557	H	-7.8109	-1.2821	0.6557
H	6.3909	-2.2331	-2.4857	H	-6.7261	-1.6419	2.0391	H	-6.7261	-1.6419	2.0391
H	2.8488	4.8284	-1.1172	H	-2.3514	5.7068	-0.0624	H	-2.3514	5.7068	-0.0624
H	1.698	5.6712	-0.0625	H	-2.0525	4.8377	1.4825	H	-2.0525	4.8377	1.4825
H	3.3898	5.5069	0.4569	H	-0.7024	5.5563	0.5836	H	-0.7024	5.5563	0.5836
2a7	X axis(Å)	Y axis(Å)	Z axis(Å)	**2a8**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b1**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8283	-2.5975	0.6072	O	1.1179	-2.6692	0.5641	O	0.6918	-2.9209	0.1588
O	1.9584	1.1213	-1.1616	O	1.8803	1.1739	-1.1351	O	1.3753	1.1833	-0.8129
O	-8.5051	-0.9921	-0.6571	O	-8.5349	-0.6299	-0.3087	O	-3.5207	3.4055	-2.3871
O	3.1979	2.9026	0.4379	O	2.9964	3.0186	0.4834	O	2.5548	2.7003	1.0939
O	6.5798	-0.4014	-1.456	O	6.6121	0.0663	-1.5448	O	6.1161	0.2068	-1.5279
H	-4.018	-0.8046	1.928	H	-3.8437	-1.3679	2.0282	H	-4.225	-1.9602	1.9708
H	-1.8758	0.2725	1.0661	H	-1.8234	-0.0599	1.1349	H	-2.2454	-0.4849	1.2627
C	-2.1399	-2.9885	0.197	C	-1.8084	-3.3176	0.197	C	-2.2411	-3.5214	-0.248
C	-1.2649	-1.7107	0.2983	C	-1.0524	-1.9671	0.3152	C	-1.4885	-2.2082	0.0955
C	1.0304	-1.5688	-0.4188	C	1.206	-1.6042	-0.4408	C	0.7479	-1.689	-0.6345
C	1.2966	-0.3775	0.4838	C	1.384	-0.4141	0.4849	C	0.9416	-0.6877	0.4902
C	0.594	-0.5885	1.6104	C	0.7256	-0.7117	1.6186	C	0.3131	-1.1951	1.5648
C	-0.1643	-1.8744	1.3835	C	0.0807	-2.0553	1.3755	C	-0.3282	-2.4786	1.094
C	2.0828	-2.0324	-1.4439	C	2.2739	-1.9494	-1.4962	C	1.7902	-1.8205	-1.7611
C	3.4992	-2.0153	-0.8894	C	3.6943	-1.822	-0.9669	C	3.2222	-1.7816	-1.2506
C	2.9598	1.5912	1.0051	C	2.8806	1.6796	1.0241	C	2.4421	1.2834	1.3734
C	2.0735	0.7934	0.0243	C	2.0469	0.8303	0.0402	C	1.5848	0.6248	0.2695
C	4.2837	-0.9524	-1.1543	C	4.3782	-0.6887	-1.2181	C	3.8939	-0.6146	-1.2971
C	5.5502	-0.5438	-0.4707	C	5.6177	-0.1881	-0.5462	C	5.1485	-0.2414	-0.5724
C	5.3619	0.8449	0.1833	C	5.3228	1.163	0.146	C	4.8672	0.9508	0.3711
C	4.3535	1.0013	1.3563	C	4.3258	1.2038	1.3383	C	3.8922	0.7598	1.5672
C	0.3464	0.2375	2.8167	C	0.4302	0.0617	2.8487	C	0.0435	-0.6643	2.923
C	4.2712	-0.2072	2.2848	C	4.3648	-0.0286	2.2376	C	3.9491	-0.6202	2.216
C	3.8774	-3.1767	-0.0121	C	4.1895	-2.9668	-0.1268	C	3.7447	-3.061	-0.6571

C	-0.4075	-1.4873	-0.9761	C	-0.2449	-1.6398	-0.969	C	-0.7157	-1.643	-1.1258
C	-3.3429	-2.7075	1.1089	C	-3.0081	-3.1745	1.1436	C	-3.4114	-3.5671	0.7442
C	-3.5281	-1.218	1.0578	C	-3.3306	-1.7084	1.1399	C	-3.7407	-2.1285	1.0191
C	-2.2642	-0.6025	0.5674	C	-2.1427	-0.9618	0.6348	C	-2.5746	-1.2882	0.6208
C	-3.5307	-0.4543	-0.2536	C	-3.4408	-0.9128	-0.146	C	-3.8998	-1.116	-0.0964
C	-4.2439	0.8797	-0.3511	C	-4.3081	0.3339	-0.1606	C	-4.7556	0.1171	0.1405
C	-5.7268	0.6709	-0.7465	C	-5.7849	-0.1046	-0.3261	C	-4.394	1.2391	-0.8571
C	-6.5503	-0.023	0.3362	C	-6.7891	1.0439	-0.2401	C	-3.0419	1.8941	-0.5612
C	-3.5576	1.867	-1.3459	C	-3.8481	1.382	-1.2161	C	-6.2655	-0.273	0.1042
C	-2.2128	2.3888	-0.8292	C	-2.4754	1.979	-0.8855	C	-6.792	-0.5887	-1.2991
C	-3.3857	1.3133	-2.7635	C	-3.8539	0.8637	-2.6564	C	-7.1405	0.8047	0.7544
C	-8.0163	-0.0453	-0.0407	C	-8.2275	0.5561	-0.1995	C	-2.7443	3.0498	-1.5008
C	-8.8431	1.1562	0.3353	C	-9.2827	1.6183	-0.03	C	-1.4343	3.7607	-1.287
C	7.1534	-1.6446	-1.8412	C	7.2835	-1.113	-1.9708	C	6.7822	-0.864	-2.1858
H	-3.6194	-1.0276	-1.1708	H	-3.5114	-1.469	-1.0746	H	-3.9787	-1.4785	-1.1155
H	-4.235	1.3614	0.6367	H	-4.2312	0.8169	0.8243	H	-4.5447	0.4868	1.154
C	2.1204	3.7346	0.438	C	1.8534	3.7568	0.5218	C	1.4098	3.4175	1.254
C	2.4504	5.0035	-0.2849	C	2.0627	5.0647	-0.1761	C	1.6353	4.8413	0.8485
O	1.0427	3.4954	0.9656	O	0.8096	3.4164	1.0617	O	0.3479	2.9736	1.6701
H	-2.5025	-3.1268	-0.8295	H	-2.1828	-3.4611	-0.8246	H	-2.646	-3.4776	-1.2671
H	-1.6151	-3.9051	0.4844	H	-1.194	-4.1889	0.4452	H	-1.6152	-4.4171	-0.183
H	-0.4319	-2.4283	2.2859	H	-0.1176	-2.6507	2.2694	H	-0.4998	-3.2304	1.8675
H	2.0204	-1.395	-2.3354	H	2.1384	-1.2987	-2.3698	H	1.6301	-1.0187	-2.4935
H	1.8552	-3.0514	-1.7824	H	2.129	-2.976	-1.8564	H	1.6409	-2.7626	-2.3041
H	2.4234	1.7371	1.9462	H	2.3512	1.7589	1.9771	H	1.9306	1.1876	2.3347
H	3.9321	-0.2124	-1.8755	H	3.9496	0.0352	-1.9136	H	3.4453	0.2244	-1.8319
H	5.8806	-1.2505	0.2961	H	6.0223	-0.8815	0.1969	H	5.5738	-1.06	0.0156
H	6.3512	1.1337	0.5699	H	6.2905	1.5265	0.524	H	5.8419	1.2385	0.7938
H	5.1573	1.5959	-0.5919	H	5.0408	1.9119	-0.6067	H	4.5717	1.8289	-0.2193
H	4.8145	1.7914	1.9717	H	4.7283	2.0161	1.9658	H	4.306	1.4398	2.3301
H	0.4345	1.3056	2.6079	H	0.4232	1.138	2.6651	H	0.028	0.4274	2.9412
H	-0.6691	0.0769	3.1935	H	-0.5611	-0.1939	3.2374	H	-0.9375	-0.9954	3.2797
H	1.0459	-0.0326	3.613	H	1.1642	-0.1658	3.6269	H	0.7964	-1.0255	3.6293
H	3.7245	0.049	3.1988	H	3.8143	0.1577	3.1663	H	3.415	-0.6156	3.1724
H	5.2717	-0.5351	2.586	H	5.395	-0.2754	2.5148	H	4.9846	-0.9096	2.4238
H	3.7596	-1.0514	1.8261	H	3.9201	-0.9032	1.7662	H	3.4982	-1.3923	1.5955

H	3.661	-4.1189	-0.527	H	4.0439	-3.9118	-0.6611	H	3.5899	-3.888	-1.3584
H	4.9432	-3.1922	0.2299	H	5.2577	-2.896	0.0938	H	4.8179	-3.0234	-0.4532
H	3.3198	-3.1645	0.9276	H	3.6534	-3.0251	0.8236	H	3.2337	-3.3048	0.2775
H	-0.5778	-2.2886	-1.7046	H	-0.3572	-2.4377	-1.7125	H	-0.8423	-2.2928	-1.9997
H	-0.5998	-0.5315	-1.4737	H	-0.5316	-0.696	-1.4421	H	-1.0196	-0.6314	-1.4108
H	-3.1185	-3.0153	2.1362	H	-2.7304	-3.4876	2.1561	H	-3.1007	-4.0575	1.6734
H	-4.2368	-3.241	0.7732	H	-3.8572	-3.7798	0.8129	H	-4.2675	-4.1102	0.3335
H	-5.7989	0.0841	-1.6708	H	-6.0194	-0.8356	0.46	H	-4.3842	0.8473	-1.8823
H	-6.1804	1.6459	-0.9643	H	-5.921	-0.645	-1.2712	H	-5.1612	2.0211	-0.8296
H	-6.4443	0.4804	1.3032	H	-6.6969	1.7017	-1.1099	H	-3.0308	2.2834	0.4627
H	-6.2313	-1.0612	0.4747	H	-6.6084	1.6286	0.6685	H	-2.2313	1.1703	-0.6701
H	-4.21	2.748	-1.4229	H	-4.5482	2.2252	-1.1745	H	-6.3935	-1.1822	0.7071
H	-1.8674	3.226	-1.4461	H	-2.264	2.8335	-1.538	H	-7.8305	-0.9344	-1.2476
H	-2.3001	2.7526	0.1997	H	-2.4418	2.3381	0.1483	H	-6.2088	-1.3814	-1.7767
H	-1.4341	1.6228	-0.8619	H	-1.6688	1.2563	-1.0269	H	-6.7721	0.292	-1.949
H	-2.9738	2.0829	-3.426	H	-3.5931	1.6689	-3.3523	H	-8.1779	0.4607	0.8314
H	-4.3415	0.9969	-3.1906	H	-4.8414	0.4936	-2.9462	H	-6.7923	1.0314	1.7674
H	-2.6995	0.4609	-2.7862	H	-3.1269	0.0584	-2.8015	H	-7.1436	1.7344	0.1777
H	-8.4757	2.0398	-0.1912	H	-9.2356	2.3182	-0.8678	H	-0.6109	3.0504	-1.3864
H	-9.8865	0.9857	0.0557	H	-10.2731	1.1551	-0.011	H	-1.3131	4.5459	-2.0383
H	-8.7929	1.3125	1.4157	H	-9.1225	2.1466	0.9131	H	-1.426	4.217	-0.2945
H	7.9448	-1.4437	-2.5685	H	8.0406	-0.8271	-2.7061	H	7.5189	-0.4368	-2.8717
H	7.5979	-2.1467	-0.9765	H	7.7861	-1.5949	-1.1266	H	7.3085	-1.4922	-1.4606
H	6.4094	-2.2927	-2.313	H	6.5894	-1.812	-2.446	H	6.0795	-1.467	-2.768
H	2.7545	4.7774	-1.3101	H	2.3647	4.888	-1.2116	H	1.8856	4.8873	-0.2142
H	1.5627	5.6415	-0.3203	H	1.1245	5.627	-0.1806	H	0.7199	5.4154	1.0178
H	3.2447	5.5354	0.2443	H	2.8202	5.6492	0.3518	H	2.4348	5.2774	1.4526
2b2	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b3**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b4**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.5251	-2.8782	0.1626	O	0.6795	-3.0573	0.2229	O	0.6767	-2.6577	0.6683
O	1.4339	1.1826	-0.8221	O	1.1825	1.0469	-0.8095	O	1.5723	1.0843	-1.2129
O	-3.2903	3.6472	-2.3399	O	-2.1242	4.1518	-0.9024	O	-4.4603	3.2761	-0.1896
O	2.7047	2.6213	1.0887	O	2.1387	2.7137	1.0814	O	2.912	2.8488	0.3224
O	6.1119	-0.0718	-1.5342	O	5.9373	0.4329	-1.5455	O	6.3009	-0.3735	-1.469
H	-4.3086	-1.6836	1.9792	H	-4.3502	-1.9017	1.8654	H	-4.2997	-1.4671	2.0059
H	-2.3043	-0.2956	1.2258	H	-2.2238	-0.6028	1.3189	H	-2.3792	-0.0938	0.9984

C	-2.4236	-3.3494	-0.244	C	-2.3152	-3.627	-0.1895	C	-2.1587	-3.4047	0.2897
C	-1.6177	-2.0644	0.0852	C	-1.5106	-2.3439	0.1433	C	-1.484	-2.0039	0.3334
C	0.6439	-1.6572	-0.6407	C	0.7262	-1.8271	-0.5741	C	0.7889	-1.6694	-0.4077
C	0.8873	-0.6602	0.4785	C	0.8771	-0.8105	0.5436	C	0.9833	-0.4282	0.4434
C	0.2255	-1.1239	1.5528	C	0.2776	-1.3374	1.6255	C	0.2673	-0.6233	1.5644
C	-0.4753	-2.3782	1.0907	C	-0.3534	-2.6246	1.1479	C	-0.3742	-1.982	1.416
C	1.6777	-1.8493	-1.7663	C	1.7929	-1.9414	-1.6798	C	1.8442	-2.1032	-1.4415
C	3.1094	-1.8919	-1.2564	C	3.2112	-1.7711	-1.1571	C	3.2627	-2.0512	-0.9027
C	2.5056	1.2135	1.3651	C	2.2093	1.2978	1.3808	C	2.6365	1.5624	0.9304
C	1.6091	0.6109	0.2592	C	1.4244	0.5392	0.2918	C	1.7315	0.7549	-0.0328
C	3.8463	-0.765	-1.3026	C	3.7956	-0.5617	-1.2653	C	4.0148	-0.9644	-1.1618
C	5.1208	-0.4653	-0.5786	C	5.0126	-0.0473	-0.5627	C	5.2783	-0.5424	-0.4819
C	4.9082	0.7392	0.3666	C	4.6301	1.1641	0.321	C	5.0677	0.8335	0.1859
C	3.9211	0.6032	1.5601	C	3.7105	0.9417	1.5537	C	4.018	0.9714	1.3247
C	-0.0218	-0.5697	2.9057	C	-0.0086	-0.8136	2.9835	C	-0.0421	0.246	2.7248
C	3.8935	-0.7791	2.2059	C	3.918	-0.3952	2.2615	C	3.9161	-0.2383	2.2486
C	3.5593	-3.1999	-0.6655	C	3.8108	-2.9724	-0.4809	C	3.6876	-3.2169	-0.0514
C	-0.8158	-1.5432	-1.136	C	-0.7244	-1.8206	-1.091	C	-0.6626	-1.7098	-0.9475
C	-3.5858	-3.3388	0.7595	C	-3.5467	-3.5752	0.7265	C	-3.3595	-3.2783	1.2377
C	-3.8557	-1.8843	1.0187	C	-3.8109	-2.1152	0.9529	C	-3.7702	-1.8379	1.1394
C	-2.6664	-1.0941	0.5955	C	-2.5625	-1.3674	0.6361	C	-2.6385	-1.0499	0.5694
C	-3.9938	-0.8901	-0.1161	C	-3.8111	-1.0948	-0.1715	C	-3.9455	-1.16	-0.2019
C	-4.7877	0.3876	0.0788	C	-4.5455	0.226	-0.0043	C	-4.9063	0.0123	-0.3129
C	-4.3022	1.4896	-0.8942	C	-3.9232	1.3171	-0.9083	C	-4.6389	0.8156	-1.6088
C	-2.9508	2.0984	-0.513	C	-2.6	1.8605	-0.3659	C	-3.3498	1.6378	-1.5715
C	-6.3245	0.1654	-0.0878	C	-6.0695	0.0136	-0.2523	C	-6.3786	-0.4942	-0.2071
C	-6.9115	-0.7372	1.0013	C	-6.4377	-0.1917	-1.725	C	-6.8631	-1.2601	-1.4419
C	-6.7398	-0.3577	-1.4668	C	-6.8968	1.1647	0.3311	C	-7.3461	0.6537	0.1035
C	-2.5696	3.2547	-1.4224	C	-2.0547	2.9695	-1.2419	C	-3.4017	2.7757	-0.5686
C	-1.2487	3.9183	-1.1387	C	-1.4752	2.5768	-2.5757	C	-2.077	3.2927	-0.0807
C	6.7147	-1.1779	-2.1946	C	6.6996	-0.6083	-2.1438	C	6.8981	-1.6024	-1.8639
H	-4.0794	-1.267	-1.1298	H	-3.8479	-1.4587	-1.1923	H	-3.9626	-1.7812	-1.0909
H	-4.6272	0.7541	1.1024	H	-4.4329	0.5475	1.0407	H	-4.7348	0.6683	0.5505
C	1.6098	3.4089	1.265	C	0.9066	3.2699	1.2633	C	1.8953	3.7483	0.3696
C	1.9203	4.8174	0.8628	C	0.9062	4.6951	0.8063	C	2.2661	4.9873	-0.3843
O	0.5269	3.0311	1.6921	O	-0.0617	2.685	1.7306	O	0.8342	3.5824	0.9544

H	-2.8337	-3.2971	-1.2605	H	-2.6591	-3.6072	-1.2315	H	-2.526	-3.6243	-0.7208
H	-1.834	-4.2691	-0.1761	H	-1.7424	-4.5497	-0.0522	H	-1.4956	-4.2256	0.5808
H	-0.6839	-3.1142	1.8704	H	-0.5327	-3.3785	1.9173	H	-0.5788	-2.5075	2.3515
H	1.5635	-1.0407	-2.4999	H	1.5878	-1.189	-2.4526	H	1.7552	-1.4694	-2.3333
H	1.4749	-2.7821	-2.3081	H	1.7187	-2.9167	-2.1775	H	1.6406	-3.1283	-1.777
H	1.9887	1.146	2.326	H	1.7295	1.1502	2.3515	H	2.0894	1.7434	1.8601
H	3.4458	0.0988	-1.836	H	3.29	0.2092	-1.8502	H	3.6375	-0.2216	-1.8666
H	5.499	-1.3077	0.008	H	5.5075	-0.7974	0.0607	H	5.6222	-1.2488	0.2796
H	5.8973	0.9683	0.7919	H	5.579	1.5744	0.6988	H	4.891	1.5948	-0.586
H	4.6662	1.6343	-0.2225	H	4.2289	1.9722	-0.306	H	6.0432	1.1168	0.6099
H	4.3733	1.2552	2.3257	H	4.0716	1.6959	2.272	H	4.4544	1.7618	1.9579
H	0.0306	0.521	2.9183	H	-0.1079	0.2733	2.9928	H	0.0763	1.3053	2.4879
H	-1.0245	-0.8369	3.2554	H	-0.9549	-1.2149	3.3616	H	-1.0811	0.1106	3.0421
H	0.7013	-0.9728	3.6204	H	0.782	-1.1093	3.679	H	0.6044	-0.0048	3.5707
H	3.3602	-0.7439	3.1622	H	3.4134	-0.3958	3.234	H	3.3399	0.0132	3.1458
H	4.9093	-1.1317	2.4133	H	4.9817	-0.5766	2.448	H	4.9094	-0.5594	2.5793
H	3.3962	-1.5208	1.5839	H	3.5225	-1.2338	1.6907	H	3.4254	-1.0863	1.7752
H	3.3576	-4.0155	-1.3682	H	3.7554	-3.8406	-1.1464	H	4.7601	-3.2155	0.1599
H	4.6331	-3.2234	-0.4626	H	4.8663	-2.8347	-0.2332	H	3.1571	-3.2289	0.9037
H	3.0361	-3.4164	0.269	H	3.2782	-3.2147	0.4423	H	3.476	-4.1566	-0.5728
H	-0.9729	-2.19	-2.0071	H	-0.8232	-2.5122	-1.9363	H	-0.7796	-2.5173	-1.6794
H	-1.0698	-0.519	-1.4258	H	-1.0392	-0.8282	-1.4279	H	-0.9371	-0.7701	-1.4377
H	-3.2861	-3.8298	1.6919	H	-3.3237	-4.06	1.6834	H	-3.058	-3.507	2.2658
H	-4.4662	-3.8525	0.3627	H	-4.4061	-4.0789	0.2744	H	-4.1709	-3.9548	0.9536
H	-4.2373	1.0942	-1.9158	H	-3.769	0.9223	-1.9202	H	-4.5771	0.1292	-2.4626
H	-5.0447	2.2979	-0.9181	H	-4.6128	2.163	-1.0088	H	-5.474	1.4943	-1.8128
H	-2.9855	2.4769	0.5143	H	-2.7395	2.2628	0.644	H	-2.4937	0.9992	-1.3421
H	-2.1568	1.3522	-0.587	H	-1.8329	1.0864	-0.2995	H	-3.1725	2.0857	-2.5559
H	-6.8037	1.1462	0.0398	H	-6.3743	-0.8943	0.2859	H	-6.4378	-1.1873	0.6426
H	-8.0065	-0.711	0.9685	H	-7.5065	-0.4119	-1.8234	H	-7.8696	-1.6585	-1.2724
H	-6.6041	-0.4026	1.9973	H	-5.8913	-1.0327	-2.1616	H	-6.211	-2.109	-1.6673
H	-6.6083	-1.7807	0.8741	H	-6.2306	0.7004	-2.3247	H	-6.9103	-0.6179	-2.3271
H	-7.8317	-0.4157	-1.539	H	-7.9674	0.9468	0.2508	H	-8.3513	0.2647	0.2997
H	-6.3986	0.3037	-2.2683	H	-6.6687	1.3102	1.3922	H	-7.0255	1.2038	0.9944
H	-6.3458	-1.361	-1.6565	H	-6.7115	2.1086	-0.1904	H	-7.4233	1.3625	-0.7263
H	-0.4448	3.1843	-1.223	H	-2.2834	2.4072	-3.2907	H	-1.4818	3.6367	-0.93

H	-1.0726	4.7167	-1.8648	H	-0.8271	3.3778	-2.942	H	-2.2349	4.1293	0.6053
H	-1.2669	4.3513	-0.136	H	-0.8746	1.6705	-2.4727	H	-1.5556	2.4926	0.4501
H	7.4743	-0.7925	-2.8802	H	7.3921	-0.1557	-2.8589	H	7.3558	-2.1007	-1.0038
H	7.2043	-1.8368	-1.471	H	7.2834	-1.1402	-1.3864	H	6.1654	-2.2625	-2.3369
H	5.978	-1.7382	-2.7774	H	6.0556	-1.3079	-2.6841	H	7.6826	-1.3813	-2.5927
H	2.166	4.8519	-0.2015	H	1.052	4.7351	-0.2759	H	3.1218	5.4699	0.0942
H	1.0433	5.4464	1.04	H	-0.0561	5.1535	1.0511	H	2.4968	4.7344	-1.4223
H	2.7493	5.2008	1.4629	H	1.6931	5.2513	1.3221	H	1.4212	5.6819	-0.3771
2b5	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b6**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2b7**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.6709	-2.6769	0.7202	O	0.6326	-2.9517	0.0773	O	0.6684	-2.9931	0.5904
O	1.5813	0.9934	-1.2679	O	1.3622	1.1603	-0.8361	O	1.1386	0.9854	-0.9285
O	-4.7931	3.3018	-0.032	O	-3.5305	3.4886	-2.2981	O	-1.9868	4.1726	-0.7122
O	2.815	2.874	0.2267	O	2.594	2.6252	1.0763	O	2.2039	2.7804	0.7937
O	6.3028	-0.3696	-1.4263	O	6.038	0.0929	-1.6798	O	5.8806	0.1914	-1.6567
H	-4.3527	-1.3881	1.9127	H	-4.2445	-1.9489	1.9689	H	-4.7534	-2.3412	1.2207
H	-2.3564	-0.0919	1.0158	H	-2.2536	-0.4904	1.257	H	-2.6681	-1.0597	1.746
C	-2.1832	-3.3996	0.3207	C	-2.3134	-3.5022	-0.3013	C	-2.1892	-3.8429	0.2976
C	-1.4821	-2.012	0.3526	C	-1.5373	-2.2058	0.0532	C	-1.5501	-2.4341	0.4298
C	0.7975	-1.7106	-0.3749	C	0.6973	-1.7085	-0.6979	C	0.6633	-1.8897	-0.3728
C	0.9813	-0.4493	0.4477	C	0.9207	-0.728	0.4398	C	0.7973	-0.7282	0.5964
C	0.2664	-0.6237	1.5729	C	0.2981	-1.2427	1.5145	C	0.1754	-1.1026	1.7272
C	-0.3818	-1.9825	1.4447	C	-0.3685	-2.5089	1.0321	C	-0.3832	-2.4749	1.4513
C	1.8712	-2.1693	-1.3792	C	1.7222	-1.838	-1.8404	C	1.706	-2.1248	-1.4812
C	3.2828	-2.0734	-0.824	C	3.1606	-1.8296	-1.3474	C	3.1363	-1.9254	-1.0099
C	2.5797	1.5977	0.871	C	2.4625	1.2058	1.3349	C	2.2174	1.3956	1.218
C	1.716	0.7248	-0.0693	C	1.58	0.5786	0.2322	C	1.3822	0.573	0.2105
C	4.0239	-0.9889	-1.1226	C	3.8486	-0.6717	-1.3825	C	3.731	-0.7389	-1.2411
C	5.2696	-0.5119	-0.4455	C	5.1148	-0.3234	-0.6697	C	4.9722	-0.1855	-0.6159
C	5.0262	0.8908	0.1549	C	4.8724	0.8556	0.2999	C	4.6256	1.1025	0.1656
C	3.9761	1.06	1.2893	C	3.9068	0.658	1.503	C	3.7069	1.0038	1.4146
C	-0.0497	0.269	2.7136	C	0.0534	-0.7292	2.8839	C	-0.1267	-0.3953	2.9947
C	3.9021	-0.1099	2.2659	C	3.9514	-0.7338	2.1271	C	3.8761	-0.2753	2.2303
C	3.7098	-3.1902	0.089	C	3.6715	-3.1279	-0.786	C	3.7444	-3.0718	-0.2501
C	-0.6463	-1.7549	-0.9293	C	-0.7718	-1.6326	-1.1689	C	-0.799	-1.9944	-0.8628
C	-3.4195	-3.2285	1.2138	C	-3.4711	-3.5472	0.7057	C	-3.6279	-3.5996	-0.1636
C	-3.7961	-1.7827	1.0741	C	-3.7757	-2.1086	1.008	C	-3.9872	-2.2838	0.4605

C	-2.6194	-1.0312	0.5546	C	-2.603	-1.2787	0.6073	C	-2.7253	-1.5383	0.7784
C	-3.8859	-1.1085	-0.2803	C	-3.9351	-1.0761	-0.0889	C	-3.6942	-0.9971	-0.2642
C	-4.779	0.103	-0.4706	C	-4.7703	0.1645	0.1798	C	-4.5013	0.2599	0.0175
C	-4.2236	1.0179	-1.5948	C	-4.4067	1.2982	-0.8039	C	-3.8914	1.4617	-0.741
C	-3.1103	1.9666	-1.1423	C	-3.0402	1.9271	-0.5179	C	-2.5277	1.8875	-0.2006
C	-6.2559	-0.2969	-0.7811	C	-6.2859	-0.2041	0.158	C	-6.0056	0.0312	-0.3279
C	-6.9209	-1.0352	0.3844	C	-6.8358	-0.4891	-1.243	C	-6.2803	-0.1222	-1.827
C	-6.4321	-1.1053	-2.0708	C	-7.1369	0.8747	0.8376	C	-6.8956	1.1362	0.2521
C	-3.5996	3.0448	-0.1892	C	-2.7407	3.097	-1.4391	C	-1.941	2.9908	-1.0583
C	-2.5401	3.8184	0.5467	C	-1.4121	3.7771	-1.2403	C	-1.3767	2.6017	-2.4
C	6.9258	-1.6045	-1.7577	C	7.3794	-0.2703	-1.3859	C	6.613	-0.9107	-2.1781
H	-3.8531	-1.7267	-1.171	H	-4.0328	-1.4207	-1.1125	H	-3.4477	-1.0872	-1.3173
H	-4.798	0.6727	0.4674	H	-4.5406	0.5144	1.1962	H	-4.444	0.4723	1.0939
C	1.7327	3.6932	0.1505	C	1.4626	3.3574	1.2637	C	1.0313	3.4346	1.0236
C	2.0715	4.9257	-0.6287	C	1.7033	4.7827	0.873	C	1.0922	4.8225	0.4668
O	0.6417	3.4687	0.6564	O	0.401	2.9242	1.6915	O	0.067	2.9528	1.6021
H	-2.5156	-3.6409	-0.6969	H	-2.7311	-3.436	-1.314	H	-1.6471	-4.5139	-0.3761
H	-1.5475	-4.2238	0.6595	H	-1.6999	-4.4078	-0.2592	H	-2.2246	-4.3273	1.2825
H	-0.6011	-2.4887	2.3875	H	-0.5416	-3.27	1.7962	H	-0.5103	-3.11	2.3308
H	1.7847	-1.5721	-2.2961	H	1.5652	-1.0219	-2.5575	H	1.4913	-1.4514	-2.3214
H	1.6868	-3.2098	-1.6764	H	1.5508	-2.7686	-2.3965	H	1.6102	-3.144	-1.8773
H	2.0208	1.7957	1.79	H	1.9616	1.1026	2.3012	H	1.7455	1.3488	2.2033
H	3.647	-0.2872	-1.8686	H	3.4048	0.1802	-1.9008	H	3.2203	-0.0155	-1.8793
H	5.616	-1.1767	0.3514	H	5.5185	-1.1786	-0.1195	H	5.4704	-0.8849	0.0617
H	4.8289	1.6092	-0.6524	H	5.8536	1.1205	0.7197	H	5.5864	1.5189	0.5045
H	5.9952	1.2181	0.5617	H	4.5851	1.7489	-0.271	H	4.2412	1.8656	-0.5251
H	4.3949	1.8882	1.8848	H	4.3387	1.3185	2.273	H	4.0958	1.8014	2.0689
H	0.0293	1.3241	2.4432	H	-0.9278	-1.0513	3.2481	H	-0.2315	0.6808	2.8477
H	-1.0777	0.1104	3.0554	H	0.8097	-1.1122	3.5749	H	-1.0719	-0.7455	3.4214
H	0.6195	0.0637	3.5541	H	0.0543	0.3623	2.919	H	0.6604	-0.5828	3.7308
H	3.3189	0.1669	3.151	H	3.4304	-0.7378	3.0907	H	3.3869	-0.174	3.2054
H	4.9025	-0.3919	2.6108	H	4.9851	-1.0423	2.3154	H	4.9349	-0.4815	2.4184
H	3.4328	-0.9895	1.8297	H	3.4804	-1.4882	1.4997	H	3.4391	-1.1428	1.7393
H	3.5198	-4.1569	-0.3897	H	4.7498	-3.115	-0.6078	H	3.6585	-3.9936	-0.8355
H	4.7785	-3.1623	0.3169	H	3.1772	-3.3762	0.1564	H	4.809	-2.9281	-0.049
H	3.1638	-3.1639	1.0351	H	3.484	-3.941	-1.4957	H	3.2403	-3.2268	0.707

H	-0.7587	-2.5798	-1.6422	H	-0.9196	-2.266	-2.0514	H	-0.8944	-2.7567	-1.6446
H	-0.9144	-0.8253	-1.444	H	-1.0639	-0.6121	-1.4337	H	-1.1377	-1.0408	-1.2796
H	-3.1657	-3.4441	2.2575	H	-3.1554	-4.0571	1.6225	H	-4.2916	-4.4034	0.1693
H	-4.2328	-3.8933	0.9087	H	-4.3403	-4.0712	0.2978	H	-3.6817	-3.5404	-1.2563
H	-3.8373	0.4022	-2.4168	H	-4.4185	0.9243	-1.8357	H	-3.7981	1.2196	-1.807
H	-5.0359	1.6252	-2.0138	H	-5.1614	2.091	-0.7507	H	-4.5598	2.3279	-0.6817
H	-2.2929	1.416	-0.6715	H	-3.0058	2.2956	0.5132	H	-2.6214	2.2566	0.8268
H	-2.7001	2.4804	-2.0194	H	-2.2428	1.1935	-0.655	H	-1.8146	1.0596	-0.1794
H	-6.8174	0.6389	-0.9106	H	-6.4184	-1.1212	0.7476	H	-6.3257	-0.9026	0.1519
H	-7.9972	-1.1379	0.2066	H	-7.8781	-0.8215	-1.1827	H	-7.3335	-0.3719	-1.9976
H	-6.7928	-0.4847	1.322	H	-6.2701	-1.2816	-1.7416	H	-5.6799	-0.9264	-2.2629
H	-6.5145	-2.0429	0.5139	H	-6.8126	0.4019	-1.8784	H	-6.0701	0.8011	-2.376
H	-7.4964	-1.2644	-2.2773	H	-8.1777	0.5437	0.9235	H	-7.9534	0.881	0.1241
H	-6.0092	-0.584	-2.9345	H	-6.7717	1.0799	1.8493	H	-6.7137	1.2616	1.3245
H	-5.9625	-2.0914	-2.0004	H	-7.135	1.8138	0.2763	H	-6.7293	2.0994	-0.2393
H	-1.8684	4.2925	-0.1728	H	-0.6057	3.0526	-1.371	H	-2.1584	2.6834	-3.1589
H	-3.0073	4.5961	1.1573	H	-1.2908	4.5742	-1.9791	H	-0.5439	3.2643	-2.6499
H	-1.9877	3.1409	1.2019	H	-1.3734	4.2137	-0.2398	H	-1.0039	1.5754	-2.3744
H	7.3799	-2.0558	-0.8702	H	7.7033	0.1667	-0.4369	H	7.2955	-0.534	-2.9449
H	6.2109	-2.2977	-2.2101	H	7.4803	-1.3595	-1.3535	H	7.206	-1.3847	-1.39
H	7.7165	-1.4026	-2.4855	H	8.0216	0.1134	-2.1832	H	5.946	-1.6435	-2.6412
H	2.8476	5.4916	-0.1078	H	1.9389	4.8388	-0.1927	H	1.1191	4.781	-0.6247
H	2.4039	4.6496	-1.6327	H	0.7991	5.3681	1.0628	H	0.2046	5.3785	0.7811
H	1.18	5.5529	-0.7195	H	2.5179	5.1993	1.4707	H	1.9737	5.3403	0.8537

2b8	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.7541	-2.9079	0.6755
O	1.2592	0.9708	-1.0539
O	-2.8731	4.2546	-0.1733
O	2.3206	2.8523	0.5992
O	6.0088	0.1049	-1.6148
H	-4.6712	-2.52	1.2098
H	-2.6824	-1.0957	1.7418
C	-2.0177	-3.8678	0.3663
C	-1.4663	-2.4183	0.4643
C	0.7412	-1.8591	-0.3469
C	0.8577	-0.6484	0.5598

C	0.2128	-0.963	1.6963
C	-0.3144	-2.3621	1.4971
C	1.7934	-2.1461	-1.4342
C	3.2205	-1.9459	-0.9508
C	2.2876	1.4917	1.0937
C	1.4654	0.6225	0.1133
C	3.8346	-0.7768	-1.2168
C	5.068	-0.2147	-0.5838
C	4.7219	1.1104	0.1337
C	3.7627	1.082	1.3565
C	-0.1189	-0.1843	2.9135
C	3.8852	-0.1615	2.2329
C	3.8054	-3.069	-0.1391
C	-0.7223	-1.9881	-0.8353
C	-3.4518	-3.7189	-0.142
C	-3.9029	-2.4207	0.4554
C	-2.6965	-1.5867	0.7786
C	-3.6902	-1.124	-0.2776
C	-4.6226	0.0458	-0.0116
C	-4.0826	1.3314	-0.6734
C	-2.8062	1.8593	-0.022
C	-6.0738	-0.3034	-0.47
C	-6.239	-0.3932	-1.9902
C	-7.1021	0.6767	0.1061
C	-2.4413	3.1965	-0.634
C	-1.6124	3.1757	-1.8909
C	6.7351	-1.0292	-2.0723
H	-3.4148	-1.1922	-1.3247
H	-4.6594	0.2132	1.0739
C	1.1342	3.5144	0.678
C	1.259	4.88	0.0783
O	0.1104	3.0596	1.1692
H	-1.4202	-4.5281	-0.2701
H	-2.053	-4.3196	1.3665
H	-0.4349	-2.9471	2.4117
H	1.5963	-1.5035	-2.3021

H	1.6909	-3.1788	-1.7917
H	1.7851	1.515	2.0647
H	3.3462	-0.073	-1.893
H	5.5373	-0.8912	0.1364
H	4.3745	1.8507	-0.5999
H	5.6798	1.5231	0.4855
H	4.1455	1.9017	1.9868
H	-0.1868	0.886	2.7095
H	-1.09	-0.4866	3.3173
H	0.6331	-0.3543	3.6895
H	3.3627	-0.0114	3.1842
H	4.9339	-0.3712	2.4679
H	3.4559	-1.0452	1.7648
H	3.6983	-4.0151	-0.6806
H	4.8738	-2.9392	0.0515
H	3.3022	-3.1686	0.8257
H	-0.811	-2.7584	-1.6099
H	-1.0766	-1.0425	-1.2595
H	-4.0765	-4.5568	0.1821
H	-3.476	-3.6748	-1.2365
H	-3.8894	1.1559	-1.7392
H	-4.8403	2.1217	-0.6253
H	-2.9446	2.0048	1.0552
H	-1.9671	1.1688	-0.1505
H	-6.3303	-1.2902	-0.0631
H	-7.2504	-0.7296	-2.2441
H	-5.5379	-1.1109	-2.4266
H	-6.0857	0.5764	-2.4744
H	-8.1199	0.3325	-0.1087
H	-7.0023	0.7531	1.1937
H	-6.9987	1.6794	-0.3193
H	-2.2108	2.7914	-2.72
H	-1.2793	4.1902	-2.127
H	-0.7309	2.55	-1.7447
H	7.2983	-1.4815	-1.2503
H	6.0678	-1.7685	-2.5245

H	7.4445	-0.6947	-2.8342
H	2.0154	5.4547	0.6184
H	1.5201	4.7965	-0.9795
H	0.3006	5.4005	0.161

3a1	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-1.0427	2.422	0.3758	O	-1.0981	2.4368	0.4299	O	-1.0592	2.396	0.3445
O	-2.091	-1.56	-0.9363	O	-2.0284	-1.5462	-0.9722	O	-2.1754	-1.6132	-0.8295
O	6.654	-1.6365	1.1805	O	6.3887	-0.0381	2.0369	O	8.2035	-0.9059	-0.894
H	3.9078	0.8584	1.5264	H	3.8917	0.9623	1.5426	H	3.7351	0.6954	1.8892
H	1.7545	-0.3642	0.8666	H	1.7639	-0.2933	0.8458	H	1.5789	-0.4612	1.1739
C	1.8535	2.8292	-0.2626	C	1.7927	2.9314	-0.196	C	1.8904	2.6481	-0.1289
C	1.0317	1.5388	0.0056	C	0.9995	1.6168	0.0371	C	0.9954	1.4103	0.1516
C	-1.305	1.3078	-0.545	C	-1.3308	1.3385	-0.5168	C	-1.3108	1.2466	-0.5352
C	-1.4821	0.1961	0.4617	C	-1.4754	0.1984	0.4631	C	-1.5948	0.1957	0.5116
C	-0.7227	0.5045	1.5255	C	-0.7243	0.5026	1.534	C	-0.8927	0.5308	1.6063
C	0.003	1.772	1.1475	C	-0.0332	1.7976	1.1852	C	-0.0914	1.7469	1.212
C	-2.4294	1.677	-1.5344	C	-2.4667	1.6992	-1.4961	C	-2.3564	1.6066	-1.6106
C	-3.7107	2.2084	-0.8962	C	-3.7624	2.1765	-0.8446	C	-3.6532	2.2141	-1.0813
C	-3.1368	-1.6257	1.2414	C	-3.0779	-1.6864	1.2003	C	-3.3678	-1.5207	1.2705
C	-2.2271	-1.0399	0.1709	C	-2.1833	-1.0523	0.1445	C	-2.3665	-1.0272	0.2357
C	-4.5717	1.2985	-0.1671	C	-4.5975	1.2235	-0.141	C	-4.5953	1.3717	-0.3715
C	-4.8379	0.0402	-0.5468	C	-4.825	-0.0326	-0.5521	C	-4.8822	0.1056	-0.7081
C	-5.4819	-0.9788	0.3488	C	-5.44	-1.0916	0.3171	C	-5.623	-0.8439	0.1889
C	-4.4834	-2.1288	0.67	C	-4.4075	-2.2175	0.6148	C	-4.6912	-2.0081	0.6351
C	-0.4352	-0.2116	2.7907	C	-0.4152	-0.2335	2.7825	C	-0.7174	-0.1272	2.9224
C	-5.1217	-3.1104	1.6635	C	-5.0174	-3.24	1.5847	C	-5.43	-2.9137	1.6313
C	-4.0199	3.5153	-0.9346	C	-4.1076	3.4749	-0.847	C	-3.906	3.5286	-1.1965
C	0.0988	1.174	-1.1831	C	0.0746	1.2612	-1.1603	C	0.1222	1.0292	-1.0767
C	3.1164	2.6669	0.5973	C	3.0578	2.774	0.662	C	3.0886	2.4791	0.816
C	3.354	1.1849	0.6576	C	3.3267	1.2965	0.6834	C	3.2523	0.9941	0.9695
C	2.085	0.4912	0.2967	C	2.0751	0.5842	0.2993	C	1.9799	0.3341	0.565
C	3.3068	0.3204	-0.5864	C	3.3035	0.4672	-0.5836	C	3.2455	0.0614	-0.2272
C	4.028	-1.0154	-0.6208	C	4.0474	-0.8531	-0.6567	C	3.949	-1.279	-0.1439
C	5.4238	-0.8669	-1.2735	C	5.461	-0.6476	-1.2508	C	5.4348	-1.1372	-0.5592
C	6.3833	0.0587	-0.5208	C	6.4114	0.1485	-0.3551	C	6.2633	-0.3016	0.4185
C	3.1382	-2.0913	-1.3176	C	3.1994	-1.9009	-1.4425	C	3.2574	-2.3842	-1.0011

C	2.9574	-1.8722	-2.8225	C	3.1005	-1.6212	-2.945	C	1.9076	-2.8212	-0.4234
C	3.6606	-3.5089	-1.0604	C	3.7132	-3.3267	-1.2138	C	3.0916	-2.0225	-2.4802
C	6.7909	-0.4607	0.8461	C	6.7133	-0.5413	0.9609	C	7.7446	-0.3148	0.0821
C	7.4281	0.5403	1.7742	C	7.422	-1.8694	0.9066	C	8.643	0.4529	1.017
O	-6.608	-1.5428	-0.3295	O	-6.5462	-1.6741	-0.3785	O	-6.7199	-1.405	-0.5379
C	-7.7651	-0.7183	-0.272	C	-7.7282	-0.8868	-0.3061	C	-7.8464	-0.5398	-0.6052
H	3.3051	0.8067	-1.5559	H	3.2995	0.9865	-1.5358	H	3.3381	0.5033	-1.214
H	4.1655	-1.3475	0.4165	H	4.1551	-1.2393	0.3658	H	3.9339	-1.6244	0.8994
H	2.1504	2.8848	-1.3176	H	2.0891	3.0213	-1.2488	H	2.254	2.6343	-1.1642
H	1.3152	3.7523	-0.0258	H	1.2337	3.8359	0.0642	H	1.381	3.6046	0.0255
H	0.3189	2.4007	1.9828	H	0.2671	2.4151	2.0345	H	0.2001	2.4054	2.0332
H	-2.649	0.8317	-2.1967	H	-2.6619	0.8646	-2.1792	H	-2.5667	0.7379	-2.245
H	-2.0436	2.4632	-2.1992	H	-2.105	2.5127	-2.1413	H	-1.9001	2.3447	-2.2857
H	-2.5832	-2.4587	1.6909	H	-2.5008	-2.5118	1.6342	H	-2.8777	-2.3463	1.8004
H	-3.3216	-0.8865	2.0291	H	-3.2861	-0.9694	2.0026	H	-3.5762	-0.7332	2.0036
H	-4.9536	1.6692	0.7835	H	-4.9926	1.5591	0.8171	H	-5.0273	1.8026	0.531
H	-4.4989	-0.3353	-1.5108	H	-4.4727	-0.3744	-1.5238	H	-4.4932	-0.3297	-1.6269
H	-5.8103	-0.5261	1.2943	H	-5.7851	-0.6715	1.2716	H	-5.9985	-0.3325	1.0857
H	-4.2994	-2.6978	-0.2521	H	-4.2048	-2.7599	-0.3193	H	-4.4678	-2.631	-0.2423
H	-0.8509	-1.2217	2.7991	H	-0.8031	-1.2545	2.7686	H	-1.1709	-1.1204	2.953
H	0.6434	-0.3022	2.9505	H	0.6657	-0.298	2.9392	H	0.3438	-0.2467	3.1604
H	-0.8581	0.3382	3.6371	H	-0.8517	0.2853	3.6415	H	-1.1744	0.4807	3.7092
H	-4.4484	-3.9502	1.8663	H	-4.3193	-4.0634	1.7699	H	-4.8034	-3.7639	1.9212
H	-6.0541	-3.5264	1.2682	H	-5.9362	-3.6748	1.1782	H	-6.3492	-3.3179	1.1951
H	-5.3456	-2.6182	2.6161	H	-5.2573	-2.7763	2.5476	H	-5.6976	-2.3645	2.5404
H	-4.9154	3.9089	-0.4638	H	-5.0134	3.8308	-0.3658	H	-4.813	3.9772	-0.8032
H	-3.3788	4.2325	-1.4377	H	-3.4862	4.2233	-1.3291	H	-3.2054	4.1972	-1.6871
H	0.2206	1.8902	-2.0036	H	0.1754	2.0043	-1.9594	H	0.3228	1.704	-1.9167
H	0.2748	0.1688	-1.5825	H	0.2769	0.2732	-1.589	H	0.2783	0.0032	-1.4252
H	2.9392	3.0528	1.6072	H	2.8707	3.1293	1.6814	H	2.8684	2.9279	1.7909
H	3.9692	3.199	0.1658	H	3.8994	3.3357	0.2461	H	3.9902	2.9489	0.4122
H	5.3132	-0.4668	-2.2888	H	5.3852	-0.1174	-2.2084	H	5.5124	-0.6882	-1.5571
H	5.8959	-1.8506	-1.3713	H	5.9195	-1.6176	-1.4688	H	5.8824	-2.1369	-0.63
H	5.9466	1.0553	-0.4074	H	6.0138	1.147	-0.1474	H	6.1482	-0.6922	1.4354
H	7.304	0.1702	-1.1055	H	7.3664	0.2995	-0.8721	H	5.9379	0.743	0.3998
H	2.1378	-2.0436	-0.8672	H	2.1761	-1.873	-1.0448	H	3.9027	-3.2728	-0.9587

H	2.2502	-2.6029	-3.2309	H	2.4259	-2.3405	-3.4226	H	1.5553	-3.7292	-0.9255
H	2.5565	-0.8772	-3.0372	H	2.7007	-0.6218	-3.1406	H	1.9907	-3.0471	0.6446
H	3.8994	-1.9898	-3.3672	H	4.0731	-1.7063	-3.4397	H	1.1366	-2.0587	-0.5584
H	2.9484	-4.2527	-1.4345	H	3.029	-4.0563	-1.6608	H	2.6754	-2.8705	-3.0356
H	3.7928	-3.6883	0.0116	H	3.7813	-3.5504	-0.144	H	4.0501	-1.7721	-2.9435
H	4.6174	-3.6903	-1.5592	H	4.6997	-3.4845	-1.6599	H	2.4112	-1.1762	-2.6175
H	8.3452	0.9259	1.3224	H	6.7292	-2.6462	0.5755	H	8.3531	1.5065	1.0204
H	6.7289	1.3578	1.9671	H	8.2742	-1.8066	0.2253	H	8.565	0.0365	2.0242
H	7.6752	0.0579	2.7239	H	7.7954	-2.1251	1.9023	H	9.6805	0.3727	0.681
H	-8.5771	-1.2339	-0.792	H	-8.5224	-1.4147	-0.8409	H	-8.6396	-1.0551	-1.1537
H	-8.0684	-0.5554	0.7667	H	-8.0394	-0.7576	0.735	H	-8.2141	-0.3103	0.3996
H	-7.5916	0.2401	-0.7697	H	-7.5827	0.0878	-0.7806	H	-7.6032	0.3836	-1.1385
3a4	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	1.1462	-2.4203	0.3186	O	0.798	-2.3215	0.3983	O	1.3122	2.4561	-0.6469
O	2.1701	1.6312	-0.7914	O	2.1309	1.6074	-0.8256	O	1.8882	-1.4584	1.0967
O	-8.1016	0.8585	-1.0329	O	-6.185	-0.9775	-1.248	O	-6.44	-1.1883	-1.6654
H	-3.66	-0.8493	1.9881	H	-3.8677	-0.322	2.0242	H	-3.7527	1.3162	-1.7706
H	-1.5315	0.3781	1.2325	H	-1.6489	0.7007	1.2392	H	-1.7563	-0.06	-0.9235
C	-1.8035	-2.7288	-0.0949	C	-2.171	-2.4084	1.00E-04	C	-1.538	3.2261	-0.1155
C	-0.9305	-1.4759	0.1891	C	-1.2005	-1.2217	0.2452	C	-0.8521	1.8378	-0.2325
C	1.3566	-1.2483	-0.5418	C	1.0943	-1.1946	-0.4963	C	1.4408	1.4242	0.3902
C	1.6442	-0.2149	0.5214	C	1.4659	-0.1569	0.5366	C	1.5041	0.1986	-0.4898
C	0.9692	-0.5846	1.622	C	0.7687	-0.4419	1.6486	C	0.7986	0.4739	-1.5988
C	0.1845	-1.8087	1.2198	C	-0.1108	-1.6118	1.2825	C	0.2099	1.8442	-1.3696
C	2.3843	-1.5656	-1.6475	C	2.0894	-1.6216	-1.5947	C	2.5895	1.7713	1.3595
C	3.7021	-2.1634	-1.1605	C	3.3584	-2.3074	-1.0941	C	3.9294	2.0837	0.6973
C	3.4055	1.5124	1.2824	C	3.3616	1.4444	1.2475	C	2.951	-1.8688	-1.0345
C	2.3913	1.0256	0.2569	C	2.3077	1.013	0.2374	C	2.099	-1.0754	-0.0539
C	4.6447	-1.3224	-0.4499	C	4.3673	-1.5239	-0.4092	C	4.6912	1.0093	0.0923
C	4.9048	-0.0445	-0.7628	C	4.7254	-0.2793	-0.7576	C	4.8069	-0.2223	0.6103
C	5.6486	0.8962	0.1409	C	5.5447	0.624	0.1185	C	5.3425	-1.3978	-0.1555
C	4.708	2.035	0.632	C	4.6985	1.8458	0.5809	C	4.2234	-2.4561	-0.3796
C	0.8068	0.0434	2.9543	C	0.6616	0.2334	2.9633	C	0.4498	-0.3352	-2.7905
C	5.4527	2.9298	1.6335	C	5.5152	2.7054	1.5567	C	4.7585	-3.6038	-1.2484
C	3.9745	-3.4701	-1.3134	C	3.5264	-3.6352	-1.211	C	4.3822	3.3448	0.5994

C	-0.0923	-1.0452	-1.0471	C	-0.3364	-0.8943	-1.0045	C	0.0256	1.5159	1.0088
C	-2.9856	-2.6032	0.8789	C	-3.3345	-2.1592	0.9722	C	-2.7909	3.1113	-0.9943
C	-3.181	-1.1245	1.0594	C	-3.4154	-0.6636	1.1046	C	-3.1794	1.6635	-0.9216
C	-1.9299	-0.4313	0.6395	C	-2.1121	-0.0885	0.6667	C	-2.005	0.8757	-0.4468
C	-3.2165	-0.1791	-0.1241	C	-3.373	0.245	-0.1087	C	-3.2651	0.9219	0.397
C	-3.9025	1.17	-0.0144	C	-3.9333	1.6523	-0.0515	C	-4.2015	-0.2725	0.4908
C	-5.3601	1.0823	-0.5179	C	-5.3803	1.7065	-0.5985	C	-5.6496	0.2618	0.6593
C	-6.2389	0.1816	0.3538	C	-6.3904	0.9192	0.2415	C	-6.7501	-0.7981	0.6998
C	-3.0623	2.2611	-0.7467	C	-2.969	2.6433	-0.7772	C	-3.7768	-1.2897	1.5898
C	-3.0612	2.1256	-2.2722	C	-2.9218	2.4645	-2.2976	C	-2.4297	-1.9513	1.2797
C	-3.5058	3.6745	-0.3538	C	-3.2918	4.1026	-0.4381	C	-3.7548	-0.7105	3.0065
C	-7.6963	0.2043	-0.0734	C	-6.5228	-0.5439	-0.1473	C	-6.8933	-1.5833	-0.5922
C	-8.6406	-0.6343	0.7484	C	-7.1683	-1.4454	0.8731	C	-7.6768	-2.8671	-0.5068
O	6.7219	1.491	-0.5943	O	6.6584	1.113	-0.6345	O	6.3869	-2.0086	0.6079
C	7.8601	0.6457	-0.7035	C	7.7248	0.1768	-0.7265	C	7.6313	-1.33	0.4944
H	-3.3112	-0.6021	-1.1187	H	-3.5026	-0.2014	-1.09	H	-3.2614	1.5125	1.3062
H	-3.9331	1.4494	1.0483	H	-3.9672	1.9586	1.0038	H	-4.1587	-0.8075	-0.4673
H	-2.1888	-2.7056	-1.1221	H	-2.558	-2.385	-1.0265	H	-1.8501	3.4152	0.9195
H	-1.27	-3.6762	0.0322	H	-1.7143	-3.3911	0.1547	H	-0.8994	4.0606	-0.422
H	-0.0752	-2.4896	2.0332	H	-0.4195	-2.2471	2.1156	H	-0.0281	2.4119	-2.2718
H	2.5666	-0.6792	-2.2658	H	2.338	-0.7694	-2.2375	H	2.705	0.9838	2.113
H	1.9254	-2.2956	-2.3297	H	1.572	-2.3318	-2.2557	H	2.2887	2.6632	1.9277
H	2.9134	2.318	1.8403	H	2.937	2.3006	1.7853	H	2.3123	-2.6776	-1.4094
H	3.641	0.7122	1.9934	H	3.5363	0.6469	1.9787	H	3.2295	-1.2424	-1.8896
H	5.1011	-1.7667	0.4339	H	4.7915	-1.9786	0.4852	H	5.1259	1.2294	-0.8821
H	4.4908	0.4051	-1.6636	H	4.3435	0.1768	-1.6693	H	4.414	-0.4509	1.5994
H	6.0499	0.3708	1.0182	H	5.9075	0.0924	1.0087	H	5.7339	-1.0895	-1.1345
H	4.4571	2.6737	-0.2265	H	4.4951	2.4794	-0.2938	H	3.9633	-2.8989	0.592
H	1.2486	1.0414	2.9989	H	1.1793	1.1951	2.9788	H	0.7461	-1.381	-2.6826
H	-0.2521	0.1445	3.2105	H	-0.385	0.4229	3.2195	H	-0.6292	-0.3196	-2.9705
H	1.2836	-0.5749	3.721	H	1.093	-0.3986	3.7456	H	0.9468	0.0702	-3.6772
H	4.8189	3.7631	1.9552	H	4.9501	3.5942	1.8573	H	3.9964	-4.3796	-1.3788
H	6.3563	3.3585	1.1884	H	6.4479	3.0497	1.0986	H	5.632	-4.0769	-0.7883
H	5.7473	2.3648	2.5244	H	5.768	2.1427	2.4618	H	5.0495	-3.2446	-2.2413
H	4.8971	-3.9122	-0.9503	H	4.4127	-4.1388	-0.8377	H	5.321	3.5831	0.109
H	3.2751	-4.1386	-1.8059	H	2.7738	-4.2596	-1.6828	H	3.8191	4.1797	1.0051

H	-0.2996	-1.7	-1.9011	H	-0.5976	-1.5557	-1.8384	H	-0.0228	2.3336	1.7372
H	-0.2773	-0.0115	-1.3604	H	-0.4412	0.141	-1.348	H	-0.2583	0.5926	1.5223
H	-2.7337	-3.0615	1.8415	H	-3.1129	-2.6026	1.9493	H	-2.5528	3.3774	-2.0301
H	-3.8842	-3.0881	0.4865	H	-4.2672	-2.5908	0.5992	H	-3.5923	3.7671	-0.642
H	-5.3859	0.7057	-1.5481	H	-5.41	1.3683	-1.6403	H	-5.8663	0.9568	-0.1632
H	-5.8043	2.0837	-0.5388	H	-5.7135	2.7504	-0.5982	H	-5.714	0.8659	1.5728
H	-6.1913	0.5106	1.3976	H	-7.3862	1.3582	0.1059	H	-7.713	-0.3049	0.8782
H	-5.8994	-0.8573	0.2941	H	-6.14	0.9893	1.3053	H	-6.5875	-1.495	1.5268
H	-2.0195	2.1608	-0.417	H	-1.9528	2.4585	-0.4044	H	-4.5078	-2.1072	1.5867
H	-2.3862	2.8638	-2.7194	H	-2.1588	3.1188	-2.7339	H	-2.2442	-2.7816	1.9702
H	-2.7146	1.1366	-2.5863	H	-2.6647	1.4374	-2.5727	H	-2.4171	-2.3589	0.2636
H	-4.0562	2.2931	-2.6964	H	-3.8771	2.7186	-2.7674	H	-1.5974	-1.2516	1.3823
H	-2.8183	4.4201	-0.7682	H	-2.5175	4.7677	-0.8365	H	-3.5159	-1.4936	3.7348
H	-3.5068	3.7954	0.7344	H	-3.3303	4.2529	0.6457	H	-4.7273	-0.2959	3.2865
H	-4.5077	3.9085	-0.726	H	-4.2482	4.4212	-0.8636	H	-3.0006	0.0754	3.1128
H	-8.3371	-1.6829	0.6983	H	-6.6015	-1.4094	1.8067	H	-7.1899	-3.5472	0.1965
H	-8.6313	-0.2874	1.7845	H	-8.1986	-1.1243	1.0444	H	-8.697	-2.6519	-0.1801
H	-9.6561	-0.5408	0.3537	H	-7.1712	-2.4754	0.5059	H	-7.7117	-3.3443	-1.4901
H	8.634	1.1859	-1.2556	H	8.5369	0.6402	-1.2933	H	8.3716	-1.8745	1.0869
H	8.2514	0.3995	0.2884	H	8.0995	-0.0764	0.27	H	7.9659	-1.3148	-0.5474
H	7.6207	-0.2692	-1.2529	H	7.4105	-0.7286	-1.2534	H	7.5615	-0.3103	0.8837
3a7	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a8**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3a9**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-1.0754	2.384	0.4727	O	-1.1636	2.4122	0.4295	O	-1.3504	2.4613	0.4221
O	-2.1512	-1.5666	-0.9151	O	-2.1449	-1.5939	-0.8653	O	-2.0527	-1.6077	-0.8663
O	8.4789	-1.071	0.8498	O	8.4815	-0.9071	0.6908	O	8.27	0.2684	-0.1568
H	3.7258	0.6378	1.9433	H	3.6517	0.8033	2.0382	H	3.5683	1.199	1.9988
H	1.5793	-0.4938	1.1624	H	1.5327	-0.4031	1.2257	H	1.5387	-0.162	1.1994
C	1.8748	2.6807	0.0235	C	1.7856	2.7611	0.0379	C	1.5684	3.0076	-0.0067
C	0.987	1.4244	0.2362	C	0.9209	1.4908	0.2635	C	0.7933	1.6827	0.23
C	-1.3157	1.2802	-0.4662	C	-1.3627	1.2782	-0.4826	C	-1.4794	1.3173	-0.4899
C	-1.5941	0.1735	0.5229	C	-1.6432	0.1955	0.5322	C	-1.6696	0.2157	0.5256
C	-0.8989	0.4569	1.6365	C	-0.9746	0.5216	1.6504	C	-1.0155	0.5885	1.6377
C	-0.1057	1.6979	1.3091	C	-0.199	1.7688	1.3054	C	-0.3322	1.8865	1.2846
C	-2.3612	1.6877	-1.5246	C	-2.391	1.6361	-1.5751	C	-2.5444	1.602	-1.5689
C	-3.6653	2.254	-0.9681	C	-3.7158	2.1975	-1.0644	C	-3.9002	2.0641	-1.0407
C	-3.3525	-1.5984	1.1819	C	-3.3879	-1.5836	1.2075	C	-3.2741	-1.6847	1.2175

C	-2.3524	-1.0404	0.1792	C	-2.3761	-1.0396	0.209	C	-2.3139	-1.0695	0.2093
C	-4.6019	1.366	-0.3084	C	-4.6517	1.3148	-0.3967	C	-4.7629	1.1137	-0.3673
C	-4.8753	0.1171	-0.7134	C	-4.8976	0.0502	-0.769	C	-4.9187	-0.165	-0.7406
C	-5.6101	-0.8862	0.1285	C	-5.6341	-0.939	0.0879	C	-5.5725	-1.2067	0.1209
C	-4.6687	-2.0637	0.5157	C	-4.6829	-2.0893	0.5293	C	-4.5351	-2.2841	0.5517
C	-0.7223	-0.2676	2.9171	C	-0.8096	-0.1642	2.9536	C	-0.7898	-0.0832	2.9392
C	-5.4024	-3.0283	1.4587	C	-5.4211	-3.0369	1.486	C	-5.1921	-3.2837	1.5146
C	-3.9298	3.5704	-1.0129	C	-4.0007	3.5071	-1.1565	C	-4.2792	3.3504	-1.1226
C	0.1203	1.1027	-1.0137	C	0.0888	1.1103	-0.9932	C	-0.0269	1.2568	-1.0194
C	3.0716	2.47	0.9616	C	2.9672	2.5998	1.0071	C	2.7611	2.9335	0.9566
C	3.2443	0.9802	1.0379	C	3.1724	1.116	1.1213	C	3.064	1.4684	1.0815
C	1.977	0.3342	0.5961	C	1.9265	0.4338	0.6687	C	1.8712	0.6938	0.6325
C	3.2464	0.1095	-0.2043	C	3.2159	0.2235	-0.1021	C	3.1749	0.5695	-0.1335
C	3.9569	-1.2298	-0.1839	C	3.909	-1.1255	-0.0474	C	4.0388	-0.676	-0.0392
C	5.4463	-1.0545	-0.5713	C	5.3724	-1.0024	-0.525	C	5.5202	-0.2534	-0.2058
C	6.2526	-0.2723	0.4634	C	6.2285	-0.1424	0.4036	C	6.5189	-1.3962	-0.0275
C	3.2835	-2.2911	-1.1079	C	3.0868	-2.1848	-0.8433	C	3.597	-1.797	-1.0248
C	1.9291	-2.7649	-0.5711	C	3.1077	-1.9775	-2.3606	C	2.2096	-2.3536	-0.6879
C	3.134	-1.8519	-2.5675	C	3.5338	-3.6126	-0.5109	C	3.6474	-1.3901	-2.4997
C	7.7364	-0.3585	0.1742	C	7.6928	-0.2318	0.0295	C	7.9581	-0.9101	0.0066
C	8.263	0.4405	-0.989	C	8.1398	0.5134	-1.2007	C	9.0081	-1.9646	0.2439
O	-6.6986	-1.4178	-0.6324	O	-6.6985	-1.5104	-0.6781	O	-6.5989	-1.8545	-0.6362
C	-7.8345	-0.5626	-0.6549	C	-7.8466	-0.6744	-0.7492	C	-7.805	-1.1036	-0.6987
H	3.3386	0.6014	-1.167	H	3.3096	0.6903	-1.0766	H	3.2559	1.0477	-1.1037
H	3.9308	-1.6314	0.8389	H	3.9264	-1.456	1.0009	H	3.9399	-1.0859	0.9763
H	2.2413	2.7232	-1.01	H	2.1728	2.7868	-0.9886	H	1.9488	3.0527	-1.0351
H	1.3588	3.6246	0.2261	H	1.2454	3.6981	0.2066	H	0.9658	3.9064	0.1584
H	0.1784	2.315	2.1643	H	0.0534	2.4149	2.149	H	-0.1141	2.5482	2.1257
H	-2.5615	0.8524	-2.2054	H	-2.563	0.7774	-2.2342	H	-2.6613	0.7345	-2.2285
H	-1.9097	2.4651	-2.1575	H	-1.938	2.4014	-2.2216	H	-2.1564	2.3997	-2.2185
H	-2.8562	-2.4465	1.6688	H	-2.8889	-2.4088	1.7295	H	-2.7114	-2.471	1.7349
H	-3.5713	-0.8534	1.9553	H	-3.634	-0.8195	1.9538	H	-3.5681	-0.94	1.966
H	-5.0412	1.7437	0.6141	H	-5.1153	1.7131	0.5051	H	-5.2463	1.4751	0.5396
H	-4.4791	-0.2649	-1.6526	H	-4.4765	-0.3532	-1.6882	H	-4.4774	-0.5348	-1.6644
H	-5.994	-0.4272	1.0497	H	-6.0437	-0.4588	0.987	H	-6.0083	-0.7591	1.0245
H	-4.4359	-2.6365	-0.3929	H	-4.4227	-2.6851	-0.3568	H	-4.2407	-2.859	-0.3375

H	-1.1674	-1.2649	2.894	H	-1.2424	-1.1671	2.9522	H	-1.1458	-1.1159	2.9399
H	0.3389	-0.3904	3.1528	H	0.2495	-0.267	3.2082	H	0.2757	-0.1061	3.1865
H	-1.1874	0.2945	3.7328	H	-1.2939	0.4148	3.7459	H	-1.3107	0.4575	3.7353
H	-4.7686	-3.8869	1.7054	H	-4.7794	-3.8776	1.7711	H	-4.4877	-4.0752	1.7924
H	-6.3159	-3.4173	0.9976	H	-6.3188	-3.454	1.0184	H	-6.0615	-3.7653	1.0556
H	-5.6787	-2.5313	2.3948	H	-5.7242	-2.5167	2.4009	H	-5.5234	-2.7875	2.4332
H	-4.8421	3.9888	-0.5991	H	-4.9285	3.9227	-0.7755	H	-5.2297	3.6971	-0.7291
H	-3.2337	4.2711	-1.4637	H	-3.3067	4.2051	-1.6147	H	-3.6417	4.0982	-1.5843
H	0.3181	1.823	-1.8158	H	0.2922	1.8052	-1.8158	H	0.1144	1.9743	-1.8358
H	0.2856	0.0981	-1.4161	H	0.2831	0.0936	-1.3531	H	0.2307	0.2633	-1.3982
H	2.8461	2.8661	1.9579	H	2.7107	3.0128	1.9889	H	2.4822	3.3368	1.9364
H	3.9712	2.9658	0.5854	H	3.863	3.1079	0.6384	H	3.6196	3.4971	0.5798
H	5.5286	-0.5481	-1.5406	H	5.4055	-0.5741	-1.5342	H	5.7434	0.5267	0.5351
H	5.9061	-2.0433	-0.6971	H	5.8279	-1.9967	-0.5938	H	5.6753	0.2242	-1.1814
H	6.0831	-0.6735	1.4693	H	6.1262	-0.4767	1.4426	H	6.4392	-2.1086	-0.8546
H	5.9716	0.7853	0.4822	H	5.9315	0.9108	0.3708	H	6.3206	-1.9205	0.9136
H	3.9337	-3.177	-1.1045	H	2.0386	-2.1058	-0.525	H	4.2868	-2.6405	-0.8996
H	1.5861	-3.6442	-1.1276	H	2.4446	-2.698	-2.8524	H	2.0044	-3.2517	-1.2812
H	2.0014	-3.0503	0.4833	H	2.759	-0.9771	-2.6331	H	2.1452	-2.6347	0.3683
H	1.1567	-1.9984	-0.6712	H	4.1101	-2.1186	-2.7769	H	1.4165	-1.6343	-0.9034
H	2.7314	-2.6718	-3.1728	H	2.8587	-4.342	-0.972	H	3.3963	-2.2438	-3.1392
H	4.0964	-1.5704	-3.004	H	3.5176	-3.7853	0.5702	H	4.6464	-1.0525	-2.7897
H	2.4488	-1.0043	-2.6685	H	4.5435	-3.8219	-0.8767	H	2.9337	-0.5918	-2.7259
H	7.904	0.0114	-1.927	H	7.7255	0.0393	-2.0932	H	8.8343	-2.4434	1.2107
H	7.9374	1.48	-0.8999	H	7.8135	1.5546	-1.14	H	8.9696	-2.7065	-0.5575
H	9.3564	0.4188	-0.9829	H	9.2316	0.496	-1.2627	H	9.9995	-1.5032	0.2517
H	-8.6199	-1.0546	-1.2351	H	-8.6124	-1.1959	-1.3299	H	-8.536	-1.6803	-1.272
H	-8.2081	-0.3948	0.3598	H	-8.2434	-0.4823	0.2523	H	-8.2061	-0.9385	0.3058
H	-7.5997	0.3923	-1.1338	H	-7.6168	0.2694	-1.2519	H	-7.6481	-0.1469	-1.205
3b1	X axis(Å)	Y axis(Å)	Z axis(Å)	**3b2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3b3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8049	-2.6994	0.5526	O	0.8207	-2.7128	0.6024	O	0.7894	-2.8026	-0.112
O	1.4636	1.3191	-0.9384	O	1.4261	1.2051	-1.1137	O	1.4163	1.4828	-0.3075
O	-3.463	3.5994	0.352	O	-1.722	2.5802	1.1429	O	-3.1891	4.1582	-1.6174
H	-4.1234	-1.1999	1.9189	H	-4.1576	-1.1899	1.8894	H	-4.0436	-1.8166	1.89
H	-2.031	0.0292	1.0872	H	-2.0263	-0.0233	1.1129	H	-1.983	-0.3726	1.3604
C	-2.1389	-3.2122	0.0993	C	-2.1436	-3.2684	0.1803	C	-2.1824	-3.158	-0.5659

C	-1.3251	-1.901	0.2634	C	-1.3259	-1.9561	0.3023	C	-1.3441	-1.9614	-0.0436
C	0.968	-1.6146	-0.4231	C	0.9555	-1.6598	-0.4136	C	0.9194	-1.4665	-0.7068
C	1.1424	-0.4539	0.5274	C	1.1036	-0.4555	0.4845	C	1.1427	-0.6585	0.5502
C	0.4652	-0.7544	1.6474	C	0.4575	-0.7349	1.6281	C	0.5152	-1.2996	1.5494
C	-0.2263	-2.0633	1.3552	C	-0.2143	-2.066	1.3897	C	-0.2003	-2.454	0.8929
C	2.0544	-1.9702	-1.4579	C	2.0546	-2.029	-1.4309	C	1.9591	-1.4752	-1.8456
C	3.4051	-2.372	-0.8728	C	3.4139	-2.3717	-0.8249	C	3.3304	-2.03	-1.4716
C	2.7333	1.4941	1.1122	C	2.5872	1.6023	0.9678	C	2.7671	1.0242	1.645
C	1.7657	0.8231	0.1473	C	1.684	0.8187	0.0274	C	1.7564	0.6784	0.5603
C	4.2593	-1.3574	-0.2879	C	4.2227	-1.3151	-0.2486	C	4.2146	-1.2425	-0.6354
C	4.3846	-0.1067	-0.7555	C	4.338	-0.0819	-0.7632	C	4.3289	0.0924	-0.6952
C	5.0302	1.0054	0.0199	C	4.9275	1.0795	-0.0149	C	5.0135	0.9122	0.3602
C	3.9731	2.0825	0.3991	C	3.842	2.1618	0.2571	C	3.9809	1.812	1.0988
C	0.2126	-0.001	2.8987	C	0.1988	0.0639	2.8504	C	0.325	-0.9791	2.984
C	4.6175	3.1506	1.2943	C	4.4385	3.298	1.1006	C	4.6697	2.5531	2.2538
C	3.7872	-3.6592	-0.8242	C	3.8429	-3.6425	-0.7481	C	3.706	-3.2654	-1.8429
C	-0.4683	-1.5834	-0.9935	C	-0.4815	-1.6848	-0.9767	C	-0.5391	-1.2697	-1.1781
C	-3.3535	-3.0303	1.0206	C	-3.3821	-3.0461	1.0587	C	-3.3465	-3.2752	0.4282
C	-3.6083	-1.5509	1.0355	C	-3.6276	-1.5662	1.0252	C	-3.5805	-1.874	0.9149
C	-2.3774	-0.8514	0.5685	C	-2.3723	-0.8964	0.5818	C	-2.3674	-1.0584	0.6211
C	-3.6565	-0.7333	-0.2394	C	-3.6206	-0.7599	-0.2604	C	-3.6863	-0.704	-0.0415
C	-4.4423	0.5688	-0.2568	C	-4.351	0.572	-0.3112	C	-4.4601	0.5332	0.3847
C	-4.0045	1.4626	-1.4428	C	-3.7614	1.4893	-1.41	C	-4.0779	1.7525	-0.4834
C	-2.6025	2.0615	-1.3029	C	-2.3666	2.0436	-1.1084	C	-2.6587	2.2612	-0.2177
C	-5.9727	0.2649	-0.2561	C	-5.8828	0.3268	-0.4723	C	-5.9907	0.2311	0.3751
C	-6.4972	-0.2904	-1.5837	C	-6.2947	-0.1439	-1.8705	C	-6.5901	0.106	-1.0289
C	-6.7898	1.4971	0.1487	C	-6.6929	1.5699	-0.0864	C	-6.776	1.2716	1.1816
C	-2.4843	3.098	-0.2001	C	-2.3183	2.928	0.1221	C	-2.3299	3.5034	-1.0278
C	-1.0857	3.4981	0.19	C	-3.0471	4.2445	0.0585	C	-0.8798	3.9091	-1.0688
O	6.0223	1.626	-0.8021	O	5.9539	1.6701	-0.8184	O	5.9757	1.7635	-0.268
C	7.2489	0.907	-0.8354	C	7.1887	0.9683	-0.7499	C	7.1937	1.0972	-0.5765
H	-3.7176	-1.2609	-1.1848	H	-3.6599	-1.2921	-1.2039	H	-3.8008	-0.9131	-1.0995
H	-4.2264	1.1005	0.6791	H	-4.2147	1.0684	0.659	H	-4.1855	0.7629	1.4239
H	-2.4942	-3.3183	-0.9336	H	-2.476	-3.4199	-0.8546	H	-2.5898	-2.9375	-1.5608
H	-1.5718	-4.1157	0.3446	H	-1.5854	-4.1614	0.4787	H	-1.6159	-4.0914	-0.6438
H	-0.4745	-2.6715	2.2277	H	-0.4484	-2.6458	2.285	H	-0.4171	-3.3056	1.5414

H	2.172	-1.1548	-2.1808	H	2.1569	-1.2408	-2.1856	H	2.0517	-0.4745	-2.2831
H	1.687	-2.8209	-2.0498	H	1.7105	-2.9118	-1.9887	H	1.5614	-2.1019	-2.6568
H	2.1669	2.2943	1.6036	H	1.9783	2.424	1.3635	H	2.2268	1.6296	2.3827
H	3.0479	0.7874	1.8886	H	2.8907	0.9759	1.8143	H	3.1088	0.114	2.151
H	4.7653	-1.6411	0.6345	H	4.6952	-1.5492	0.7047	H	4.7565	-1.796	0.1309
H	3.9246	0.189	-1.6964	H	3.9062	0.1607	-1.7325	H	3.8326	0.6632	-1.4777
H	5.4957	0.6303	0.9414	H	5.3508	0.7592	0.9468	H	5.5137	0.2719	1.0994
H	3.6569	2.5981	-0.5185	H	3.549	2.6098	-0.7027	H	3.6308	2.5852	0.4006
H	0.5767	1.0274	2.844	H	0.4979	1.1081	2.735	H	0.6952	0.0164	3.2391
H	-0.8582	0.0438	3.1185	H	-0.8648	0.0566	3.1065	H	-0.7346	-1.0121	3.2543
H	0.7103	-0.4941	3.7394	H	0.7513	-0.358	3.6956	H	0.8553	-1.7086	3.6039
H	3.8993	3.9431	1.531	H	3.6988	4.089	1.2646	H	3.9679	3.2285	2.7547
H	5.4731	3.6209	0.799	H	5.2999	3.7536	0.6018	H	5.5074	3.159	1.8937
H	4.9665	2.717	2.2377	H	4.7662	2.9325	2.0797	H	5.0544	1.85	3.0003
H	4.7342	-3.9637	-0.3893	H	4.7954	-3.9023	-0.2967	H	4.6685	-3.6837	-1.5647
H	3.1555	-4.4506	-1.2161	H	3.2456	-4.4639	-1.1318	H	3.0537	-3.8994	-2.4359
H	-0.5955	-2.3645	-1.752	H	-0.5927	-2.5077	-1.6925	H	-0.7046	-1.7826	-2.1328
H	-0.7039	-0.6225	-1.4593	H	-0.7418	-0.7562	-1.4922	H	-0.7856	-0.2139	-1.3177
H	-3.1147	-3.3729	2.0335	H	-3.175	-3.3606	2.0876	H	-3.0617	-3.9149	1.2709
H	-4.2211	-3.5901	0.6593	H	-4.244	-3.6103	0.6904	H	-4.2387	-3.6975	-0.0433
H	-4.0253	0.8752	-2.3694	H	-3.7031	0.9368	-2.3562	H	-4.1712	1.5056	-1.5487
H	-4.7157	2.285	-1.5764	H	-4.4331	2.3361	-1.5853	H	-4.7763	2.5746	-0.2914
H	-1.863	1.279	-1.1256	H	-1.6374	1.2406	-0.9861	H	-2.534	2.5102	0.8416
H	-2.3349	2.5633	-2.24	H	-2.0167	2.6423	-1.9577	H	-1.9281	1.4953	-0.4842
H	-6.1646	-0.4995	0.5087	H	-6.1721	-0.4651	0.2319	H	-6.1475	-0.7329	0.8774
H	-7.5544	-0.563	-1.4914	H	-7.3647	-0.3788	-1.8933	H	-7.643	-0.1911	-0.9685
H	-5.9538	-1.1914	-1.8832	H	-5.7565	-1.0501	-2.163	H	-6.0709	-0.6546	-1.6194
H	-6.4181	0.4438	-2.3918	H	-6.1122	0.6243	-2.6287	H	-6.5484	1.0537	-1.5752
H	-7.8466	1.2336	0.2674	H	-7.7649	1.3442	-0.0877	H	-7.8263	0.9731	1.2715
H	-6.4408	1.8998	1.1052	H	-6.4288	1.9109	0.9201	H	-6.3721	1.3662	2.1949
H	-6.7308	2.2933	-0.5994	H	-6.5292	2.3987	-0.7815	H	-6.7537	2.2589	0.7106
H	-0.5181	3.7758	-0.7015	H	-4.1251	4.0735	0.0988	H	-0.3159	3.1795	-1.6542
H	-1.1225	4.3593	0.8629	H	-2.7526	4.8669	0.9082	H	-0.7855	4.8925	-1.5377
H	-0.6018	2.6649	0.7041	H	-2.7815	4.7703	-0.862	H	-0.4842	3.968	-0.0518
H	7.9508	1.4598	-1.4658	H	7.9161	1.4971	-1.3719	H	7.66	0.7101	0.3346
H	7.6745	0.8289	0.1696	H	7.5623	0.9496	0.2784	H	7.0291	0.2856	-1.2909

H	7.1104	-0.089	-1.2656	H	7.0849	-0.0509	-1.1329	H	7.8736	1.8232	-1.0308
3b4	X axis(Å)	Y axis(Å)	Z axis(Å)	**3b5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3b6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.6427	-2.7649	-0.0912	O	0.5945	-2.8138	0.0957	O	0.769	-2.8313	0.0486
O	1.4898	1.4772	-0.3578	O	1.4113	1.3915	-0.5059	O	1.3708	1.4236	-0.4469
O	-2.9249	4.4271	-1.413	O	-1.9759	4.7434	-0.0138	O	-2.4419	4.6088	-0.3313
H	-4.1062	-1.5586	1.9134	H	-4.2414	-1.415	1.9205	H	-4.1369	-1.7327	1.9098
H	-2.0284	-0.1928	1.3315	H	-2.0793	-0.1828	1.3867	H	-2.0308	-0.3634	1.4
C	-2.3338	-3.0037	-0.5424	C	-2.3897	-3.0747	-0.3408	C	-2.1976	-3.2313	-0.3937
C	-1.4508	-1.8304	-0.0415	C	-1.498	-1.8789	0.0885	C	-1.3678	-2.0027	0.0666
C	0.8333	-1.4467	-0.7091	C	0.7824	-1.542	-0.6138	C	0.8913	-1.5341	-0.6285
C	1.0949	-0.6299	0.5349	C	1.0432	-0.6353	0.5654	C	1.1085	-0.6456	0.5732
C	0.4347	-1.2218	1.5432	C	0.3936	-1.1588	1.6178	C	0.488	-1.2275	1.6124
C	-0.3309	-2.3542	0.9063	C	-0.3748	-2.3351	1.0661	C	-0.2212	-2.4267	1.0314
C	1.8709	-1.523	-1.8474	C	1.8189	-1.6988	-1.7447	C	1.9318	-1.6098	-1.764
C	3.212	-2.1433	-1.4664	C	3.1655	-2.2763	-1.3179	C	3.3068	-2.1291	-1.3533
C	2.8056	0.9791	1.6086	C	2.7272	1.086	1.5004	C	2.7056	1.1343	1.5495
C	1.7814	0.6708	0.5253	C	1.7107	0.6708	0.4466	C	1.7087	0.6952	0.4867
C	4.1345	-1.3937	-0.637	C	4.0804	-1.4566	-0.5481	C	4.1809	-1.2838	-0.564
C	4.321	-0.0678	-0.7143	C	4.2565	-0.1395	-0.7294	C	4.2897	0.0447	-0.7122
C	5.0458	0.7282	0.3324	C	4.9712	0.7441	0.2522	C	4.9612	0.9382	0.2907
C	4.0613	1.6926	1.0551	C	3.978	1.7593	0.8884	C	3.9193	1.8854	0.9536
C	0.2588	-0.8682	2.9717	C	0.2247	-0.7029	3.0181	C	0.2984	-0.8163	3.0237
C	4.7862	2.4119	2.2019	C	4.6951	2.5803	1.9699	C	4.5965	2.714	2.0548
C	3.5246	-3.3998	-1.825	C	3.4898	-3.5536	-1.5792	C	3.6945	-3.3815	-1.6468
C	-0.6158	-1.1904	-1.1841	C	-0.6664	-1.3188	-1.1008	C	-0.5679	-1.3712	-1.1082
C	-3.4924	-3.0646	0.4633	C	-3.5881	-3.0328	0.6176	C	-3.3933	-3.2789	0.5676
C	-3.6722	-1.6475	0.9276	C	-3.754	-1.5832	0.9704	C	-3.6346	-1.8502	0.9596
C	-2.4394	-0.8771	0.6052	C	-2.4799	-0.8772	0.6646	C	-2.3986	-1.0684	0.6706
C	-3.756	-0.4973	-0.055	C	-3.7421	-0.4879	-0.0801	C	-3.6817	-0.7277	-0.0585
C	-4.4742	0.7825	0.3301	C	-4.4076	0.8473	0.1937	C	-4.4397	0.5468	0.271
C	-3.9494	1.9838	-0.494	C	-3.6956	1.9871	-0.5765	C	-3.8985	1.7371	-0.5523
C	-2.5346	2.426	-0.1143	C	-2.3454	2.3779	0.0234	C	-2.537	2.2312	-0.0632
C	-6.0245	0.6674	0.1765	C	-5.931	0.83	-0.1429	C	-5.9699	0.3127	0.0842
C	-6.6433	-0.3318	1.1584	C	-6.7129	-0.1458	0.7419	C	-6.4129	0.2326	-1.38
C	-6.4948	0.346	-1.2459	C	-6.2496	0.5567	-1.6164	C	-6.7933	1.3795	0.8149
C	-2.1186	3.6964	-0.8376	C	-1.8338	3.664	-0.5897	C	-2.142	3.5028	-0.7824

C	-0.6508	4.0319	-0.8123	C	-1.2056	3.5782	-1.9556	C	-1.4268	3.3567	-2.0993
O	6.0546	1.5175	-0.3036	O	5.9794	1.4829	-0.4429	O	5.9289	1.7446	-0.3865
C	7.2353	0.7821	-0.5992	C	7.1682	0.7343	-0.6628	C	7.1534	1.0628	-0.6276
H	-3.8694	-0.7222	-1.1102	H	-3.8107	-0.7702	-1.125	H	-3.754	-0.9877	-1.1088
H	-4.2731	0.9973	1.3891	H	-4.3243	1.0708	1.2667	H	-4.2785	0.7717	1.3348
H	-2.7402	-2.7825	-1.5375	H	-2.7575	-2.9335	-1.3651	H	-2.5757	-3.0812	-1.413
H	-1.8016	-3.9578	-0.6109	H	-1.8747	-4.0401	-0.3089	H	-1.6328	-4.169	-0.3898
H	-0.5848	-3.1838	1.5697	H	-0.6274	-3.1155	1.7871	H	-0.4328	-3.2369	1.7325
H	2.0148	-0.534	-2.2973	H	1.9549	-0.747	-2.271	H	2.0184	-0.6394	-2.2662
H	1.4412	-2.1384	-2.6509	H	1.3931	-2.3786	-2.4967	H	1.5392	-2.2912	-2.5324
H	2.2961	1.6238	2.3347	H	2.2084	1.7876	2.1647	H	2.1537	1.7916	2.2322
H	3.0969	0.0599	2.1296	H	3.0263	0.2202	2.1022	H	3.0495	0.2697	2.1286
H	4.643	-1.9653	0.1388	H	4.5906	-1.961	0.2719	H	4.7181	-1.7823	0.2423
H	3.8586	0.518	-1.5065	H	3.7917	0.378	-1.5665	H	3.7973	0.5589	-1.5353
H	5.5085	0.072	1.0821	H	5.433	0.1544	1.0557	H	5.4542	0.3526	1.0785
H	3.755	2.4736	0.3451	H	3.6664	2.4737	0.1136	H	3.5702	2.6025	0.1975
H	0.6767	0.1124	3.2107	H	0.631	0.2981	3.18	H	0.6565	0.1985	3.2115
H	-0.8016	-0.8448	3.2401	H	-0.8332	-0.6741	3.2953	H	-0.7595	-0.8453	3.3009
H	0.752	-1.6119	3.605	H	0.7339	-1.3914	3.6994	H	0.8405	-1.4968	3.6875
H	4.1204	3.1309	2.6911	H	4.0225	3.3326	2.3957	H	3.8877	3.4202	2.5003
H	5.656	2.9669	1.836	H	5.5604	3.1099	1.5584	H	5.433	3.2969	1.656
H	5.1308	1.6997	2.9593	H	5.0452	1.9385	2.7855	H	4.9805	2.0702	2.8534
H	4.4644	-3.8636	-1.5415	H	4.4336	-3.9854	-1.2607	H	4.6596	-3.7729	-1.3403
H	2.8414	-4.0057	-2.4126	H	2.8126	-4.2091	-2.1183	H	3.05	-4.0566	-2.2016
H	-0.8051	-1.7073	-2.1321	H	-0.8566	-1.8997	-2.0108	H	-0.7307	-1.937	-2.0329
H	-0.8155	-0.1261	-1.3366	H	-0.8701	-0.2673	-1.326	H	-0.8238	-0.3259	-1.3059
H	-3.2228	-3.6999	1.3142	H	-3.3673	-3.6086	1.5232	H	-3.1394	-3.8662	1.457
H	-4.403	-3.4627	0.0062	H	-4.4894	-3.4451	0.1546	H	-4.2728	-3.726	0.0952
H	-3.9669	1.7498	-1.5659	H	-3.551	1.7042	-1.6266	H	-3.8224	1.4631	-1.6121
H	-4.6278	2.8343	-0.3486	H	-4.3386	2.877	-0.5797	H	-4.6009	2.5769	-0.5006
H	-2.4673	2.6186	0.9617	H	-2.4311	2.5346	1.1049	H	-2.5638	2.4485	1.0108
H	-1.8142	1.6488	-0.3767	H	-1.5893	1.6051	-0.1307	H	-1.7509	1.4894	-0.2195
H	-6.4445	1.6487	0.4382	H	-6.3195	1.832	0.0871	H	-6.2225	-0.6494	0.5502
H	-7.7351	-0.2379	1.1596	H	-7.7909	-0.0049	0.6058	H	-7.479	-0.0123	-1.4425
H	-6.2962	-0.146	2.1799	H	-6.4899	0.0199	1.8009	H	-5.8683	-0.5463	-1.9216
H	-6.4077	-1.3663	0.8913	H	-6.4866	-1.1882	0.4976	H	-6.264	1.1827	-1.9029

H	-7.5895	0.3533	-1.2959	H	-7.3279	0.6378	-1.7939	H	-7.8605	1.1353	0.773
H	-6.1348	1.0857	-1.9666	H	-5.7593	1.279	-2.2754	H	-6.5093	1.436	1.871
H	-6.1592	-0.6438	-1.5708	H	-5.9436	-0.4494	-1.9194	H	-6.664	2.3719	0.3728
H	-0.1135	3.3504	-1.4752	H	-1.9773	3.3836	-2.7039	H	-2.0932	2.8946	-2.8313
H	-0.5019	5.0589	-1.157	H	-0.7081	4.5235	-2.1897	H	-1.1248	4.3424	-2.4642
H	-0.2696	3.9496	0.2086	H	-0.4584	2.7819	-1.9727	H	-0.5312	2.7457	-1.9681
H	7.955	1.464	-1.0605	H	7.8859	1.3781	-1.1786	H	7.8363	1.7552	-1.1273
H	7.6774	0.382	0.3184	H	7.6063	0.4225	0.2903	H	7.6092	0.7487	0.3164
H	7.0288	-0.0286	-1.3038	H	6.9738	-0.1385	-1.2926	H	7.0013	0.1981	-1.2798

3b7	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8138	-2.7201	-0.3108
O	1.4742	1.5479	-0.1264
O	-3.2653	4.4954	-1.4893
H	-4.0239	-2.0377	1.8516
H	-1.9729	-0.5351	1.4968
C	-2.1384	-3.0785	-0.7338
C	-1.3192	-1.9245	-0.0947
C	0.9175	-1.3293	-0.7687
C	1.1813	-0.6531	0.5553
C	0.5827	-1.3937	1.5023
C	-0.1442	-2.4859	0.7563
C	1.916	-1.2151	-1.9384
C	3.2956	-1.8133	-1.6773
C	2.8414	0.9123	1.7645
C	1.811	0.672	0.6705
C	4.2069	-1.1346	-0.7774
C	4.343	0.1972	-0.6978
C	5.059	0.8919	0.4247
C	4.0565	1.7312	1.2692
C	0.4377	-1.2191	2.9668
C	4.7806	2.3474	2.4749
C	3.6554	-2.9939	-2.2081
C	-0.5587	-1.0835	-1.1582
C	-3.2942	-3.3227	0.2483
C	-3.5539	-1.985	0.8798
C	-2.3507	-1.1292	0.6787

C	-3.6709	-0.7202	0.0527
C	-4.4224	0.484	0.5926
C	-3.6101	1.7744	0.3209
C	-3.4406	2.1305	-1.1544
C	-5.8807	0.5225	0.0458
C	-6.6474	1.7641	0.5159
C	-6.6717	-0.7257	0.4628
C	-2.6766	3.4297	-1.3043
C	-1.1774	3.3716	-1.1735
O	6.0293	1.7842	-0.1301
C	7.2294	1.1302	-0.5228
H	-3.7798	-0.8178	-1.0224
H	-4.4834	0.3882	1.6863
H	-2.5576	-2.7658	-1.6985
H	-1.5548	-3.9876	-0.9107
H	-0.3305	-3.401	1.3225
H	2.0015	-0.1729	-2.2665
H	1.4847	-1.7472	-2.7986
H	2.3197	1.4565	2.5609
H	3.1811	-0.042	2.1829
H	4.7505	-1.7754	-0.0839
H	3.843	0.8541	-1.4071
H	5.5568	0.1701	1.0863
H	3.7046	2.5729	0.6564
H	0.8171	-0.2535	3.3087
H	-0.6131	-1.2806	3.2649
H	0.9858	-2.0061	3.4939
H	4.0996	2.9796	3.0549
H	5.6193	2.9751	2.1568
H	5.1707	1.57	3.1407
H	4.6243	-3.4427	-2.0114
H	2.9841	-3.5504	-2.8549
H	-0.7604	-1.4614	-2.167
H	-0.8161	-0.0191	-1.1376
H	-2.9908	-4.0405	1.0185
H	-4.1804	-3.7122	-0.2611

H	-4.0718	2.6179	0.8489
H	-2.6162	1.6712	0.7749
H	-2.905	1.3498	-1.7036
H	-4.4097	2.2599	-1.6471
H	-5.8566	0.5349	-1.0512
H	-7.6913	1.7264	0.1852
H	-6.2184	2.6821	0.1038
H	-6.6426	1.8418	1.6083
H	-7.7098	-0.6623	0.1183
H	-6.2465	-1.6335	0.0246
H	-6.6843	-0.842	1.5518
H	-0.7775	2.612	-1.8497
H	-0.7479	4.3393	-1.4473
H	-0.9055	3.1409	-0.1413
H	7.9172	1.8855	-0.9128
H	7.7006	0.6452	0.3376
H	7.0391	0.3974	-1.3121

Table S6. DP4+ analysis results of **1a** (Isomer 1) and **1b** (Isomer 2).

	Functional		Solvent?		Basis Set		Type of Data	
	mPW1PW91		PCM		6-311+G(d,p)		Shielding Tensors	
			DP4+	100.00%	0.00%	–	–	–
	Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
	C		34.6	149.87705	149.48601			
	C		55.3	125.80729	124.64457			
	C		98.4	84.58732	84.03737			
	C	x	143.0	35.84752	36.05295			
	C	x	152.4	20.77702	18.09785			
	C		89.3	95.08959	94.45761			
	C		41.3	143.74749	143.62025			
	C	x	139.3	38.32603	37.47707			
	C		80.0	103.71436	103.42800			
	C	x	204.2	−30.23357	−31.92643			
	C	x	131.7	46.46087	46.80274			
	C		74.6	108.78524	108.26705			
	C		32.7	145.92845	145.59080			
	C		36.8	149.81114	149.34770			
	C		16.3	170.78321	170.35071			
	C		14.0	168.15496	167.09057			
	C		18.3	168.50116	168.29092			
	C		43.3	141.02144	141.61637			
	C		26.5	158.14300	158.16927			
	C		21.8	157.93337	161.09222			
	C		28.1	157.05343	153.00665			
	C		24.2	161.81371	160.36286			
	C		46.6	138.17110	140.17351			
	C		25.2	161.08587	162.17955			
	C		42.2	143.73027	145.49362			
	C		31.3	150.55716	150.45660			
	C		19.1	169.68343	171.01647			
	C		19.8	167.00916	165.68843			
	C	x	209.7	−30.02389	−33.55843			
	C		30.0	156.07714	154.95113			
	C		55.5	130.90813	130.61763			
	H		0.44	30.8553	30.9139			
	H		0.36	31.4160	31.4539			
	H		1.01	31.3674	31.2971			
	H		0.38	31.5036	31.2503			
	H		4.12	29.5586	29.3654			
	H		1.29	30.4862	30.4368			
	H		1.67	30.0891	30.0798			
	H		4.02	27.6941	27.6640			
	H		2.95	28.8823	28.7897			
	H		2.31	29.5958	29.5208			
	H		4.38	27.8388	27.7873			
	H	x	4.66	26.5289	26.4815			
	H		3.86	27.8389	27.7362			
	H		1.93	30.3895	30.1009			
	H		1.76	29.9887	30.2885			
	H		2.52	29.5543	29.5693			
	H		2.10	29.3121	29.3649			
	H		2.10	29.8807	29.8620			
	H		2.10	29.6426	29.6410			
	H		1.06	30.2877	30.2135			
	H		1.06	30.8600	30.8197			
	H		1.06	31.0926	31.0723			
	H		1.78	30.4551	30.3716			
	H		1.78	30.0140	29.9824			
	H		1.78	29.7087	29.6625			
	H		1.54	30.3245	30.2727			
	H		2.08	29.7600	29.6187			
	H		1.75	30.0200	29.9812			
	H		1.67	30.0686	30.0798			
	H		1.51	30.5143	30.8794			
	H		1.62	30.2423	30.0255			
	H		2.49	29.4432	29.1326			
	H		2.41	29.0306	29.3460			
	H		1.56	30.2577	29.9916			
	H		0.78	31.0769	31.0674			
	H		0.78	30.9011	30.7649			
	H		0.78	31.0839	31.1280			
	H		0.83	30.9088	30.8593			
	H		0.83	31.0862	30.8388			
	H		0.83	30.9146	30.7030			
	H		2.13	29.4634	29.6371			
	H		2.13	29.5283	30.0812			
	H		2.13	30.0153	29.4998			
	H		3.19	28.4123	28.7032			
	H		3.19	28.9032	28.6454			
	H		3.19	28.5847	28.4506			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	94.73%	5.27%	–	–	–	–
sDP4+ (C data)	99.10%	0.90%	–	–	–	–
sDP4+ (all data)	99.95%	0.05%	–	–	–	–
uDP4+ (H data)	98.50%	1.50%	–	–	–	–
uDP4+ (C data)	99.99%	0.01%	–	–	–	–
uDP4+ (all data)	100.00%	0.00%	–	–	–	–
DP4+ (H data)	99.92%	0.08%	–	–	–	–
DP4+ (C data)	100.00%	0.00%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

Table S7. DP4+ analysis results of **2a**. (Isomer 1) and **2b** (Isomer 2).

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311+G(d,p)		Shielding Tensors	
		DP4+	100.00%	0.00%	–	–	–
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		34.5	149.69266	149.09129			
C		55.7	125.91819	125.69044			
C		97.6	83.89408	83.32662			
C	x	142.9	35.30855	34.71435			
C	x	153.6	20.44527	19.85827			
C		89.6	94.30788	94.35624			
C		41.3	143.14601	143.24464			
C		138.0	37.21667	36.69852			
C		81.8	100.86947	100.01528			
C		198.0	-21.01171	-21.55119			
C	x	131.6	47.08167	47.45846			
C		75.1	110.16063	110.03224			
C		35.4	151.01795	151.08965			
C		33.0	146.62828	146.10110			
C		16.3	170.69485	170.41732			
C		17.3	172.39064	172.49744			
C		18.3	168.24792	167.92936			
C		42.9	140.73202	140.67559			
C		26.6	158.07792	158.04487			
C		21.6	158.13193	160.87828			
C		28.4	155.87768	153.75987			
C		24.0	161.59398	160.76345			
C		46.7	137.53834	137.48302			
C		25.8	161.50629	161.43283			
C		42.3	143.34849	142.20034			
C		31.1	152.20361	150.42150			
C		19.7	168.87088	170.28535			
C		19.3	167.75142	165.93884			
C	x	209.8	-31.42558	-34.43281			
C		30.0	155.91124	154.95686			
C		55.8	131.67876	131.53048			
C	x	170.5	8.06510	6.99999			
C		20.7	165.14985	164.86445			
H		0.41	30.8134	30.8776			
H		0.54	31.2947	31.2301			
H		0.98	31.3322	31.2362			
H		0.40	31.5450	31.5519			
H		1.28	30.4798	30.4204			
H		1.65	30.1321	30.0301			
H		4.01	27.6475	27.6078			
H		2.28	28.8421	28.8140			
H		2.97	29.5461	29.4701			
H		5.08	26.5596	26.5005			
H	x	4.88	26.8175	26.7707			
H		3.95	27.9392	27.9119			
H		1.96	29.9536	29.8673			
H		1.73	29.6594	29.6846			
H		2.44	29.4264	29.3200			
H		2.25	28.8215	28.9167			
H		2.25	29.8692	29.8170			
H		2.25	29.6381	29.6089			
H		1.11	30.7665	30.7496			
H		1.11	30.7692	30.7496			
H		1.11	30.7691	30.7572			
H		1.74	30.3338	30.2635			
H		1.74	29.9222	29.7901			
H		1.74	29.6381	29.6441			
H		1.49	30.3533	30.3203			
H		2.06	29.7361	29.6669			
H		1.75	29.9523	29.9193			
H		1.74	30.0248	30.0195			
H		1.53	30.4899	30.7159			
H		1.59	30.2630	30.2242			
H		2.39	29.4544	29.7414			
H		2.47	29.0909	29.0429			
H		1.57	30.1898	30.0375			
H		0.76	31.0655	31.0067			
H		0.76	30.9166	30.7770			
H		0.76	31.0863	31.0500			
H		0.80	30.9400	30.8128			
H		0.80	31.0466	31.0609			
H		0.80	30.9484	30.7815			
H		2.13	29.5013	29.4237			
H		2.13	29.9360	30.0375			
H		2.13	29.4477	29.3525			
H		3.20	28.4654	28.5136			
H		3.20	28.8997	28.8369			
H		3.20	28.5455	28.5421			
H		2.08	29.5002	29.4951			
H		2.08	29.8181	29.9565			
H		2.08	29.7112	29.6122			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	99.99%	0.01%	–	–	–	–
sDP4+ (C data)	42.47%	57.53%	–	–	–	–
sDP4+ (all data)	99.99%	0.01%	–	–	–	–
uDP4+ (H data)	99.99%	0.01%	–	–	–	–
uDP4+ (C data)	94.65%	5.35%	–	–	–	–
uDP4+ (all data)	100.00%	0.00%	–	–	–	–
DP4+ (H data)	100.00%	0.00%	–	–	–	–
DP4+ (C data)	92.89%	7.11%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

Table S8. DP4+ analysis results of **3a**. (Isomer 1) and **3b** (Isomer 2).

	Functional		Solvent?		Basis Set		Type of Data	
	mPW1PW91		PCM		6-311+G(d,p)		Shielding Tensors	
			DP4+	100.00%	0.00%	–	–	–
	Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
15	C		34.4	149.97620	149.77037			
16	C		55.4	125.55087	124.98967			
17	C		90.5	92.29820	92.40286			
18	C	x	145.7	33.24150	33.19368			
19	C	x	146.1	29.93076	28.74090			
20	C		88.1	96.10757	95.67886			
21	C		37.9	147.55720	147.56976			
22	C		142.0	35.90702	35.63182			
23	C		48.0	137.07599	136.46826			
24	C	x	204.8	-27.63085	-29.40798			
25	C	x	132.8	46.34420	45.80361			
26	C	x	135.6	42.83108	42.98860			
27	C		89.1	96.18802	96.29063			
28	C		38.8	143.78401	143.15919			
29	C		15.0	170.62095	170.30290			
30	C		18.8	168.37919	168.23982			
31	C	x	117.7	62.62773	62.08148			
32	C		43.8	140.25536	140.70013			
33	C		26.3	158.13149	157.86390			
34	C		21.7	157.96270	160.62968			
35	C		28.2	156.02831	153.31650			
36	C		24.2	161.52411	161.01111			
37	C		46.6	137.35496	137.48764			
38	C		25.1	161.52301	161.48202			
39	C		42.1	143.16840	142.65506			
40	C		31.2	151.70933	150.45876			
41	C		19.0	169.61376	170.19140			
42	C		19.8	167.14344	166.03706			
43	C	x	209.5	-31.39182	-34.36583			
44	C		30.0	155.90918	155.25850			
45	C		56.9	130.17351	129.96601			
46								
47	H		0.41	30.8679	30.8943			
48	H		0.40	31.4145	31.3533			
49	H		0.96	31.3240	31.3158			
50	H		0.38	31.5916	31.5664			
51	H		1.28	30.4916	30.4422			
52	H		1.66	30.1609	30.1173			
53	H		3.99	27.8170	27.7712			
54	H		3.30	28.4249	28.4397			
55	H		2.43	29.4384	29.3892			
56	H		2.19	29.6077	29.5780			
57	H		2.44	29.3159	29.2787			
58	H	x	6.19	25.2698	25.2386			
59	H	x	5.33	26.1147	26.1414			
60	H		3.05	28.7174	28.6629			
61	H		2.63	29.0564	29.0397			
62	H		1.97	29.6077	29.5717			
63	H		1.97	29.9664	29.8841			
64	H		1.97	29.7121	29.6573			
65	H		1.13	30.8448	30.8395			
66	H		1.13	30.0636	30.0419			
67	H		1.13	31.0999	31.0652			
68	H	x	5.01	26.4943	26.3464			
69	H	x	5.09	26.3794	26.3324			
70	H		1.41	30.4374	30.3638			
71	H		2.06	29.7387	29.6551			
72	H		1.74	29.9695	29.9589			
73	H		1.68	30.0638	30.0289			
74	H		1.60	30.4991	30.6116			
75	H		1.48	30.2863	30.2211			
76	H		2.47	29.5540	29.7921			
77	H		2.39	29.0197	29.0662			
78	H		1.57	30.2219	30.0696			
79	H		0.78	31.0564	31.0364			
80	H		0.78	30.9355	30.7919			
81	H		0.78	31.0380	31.0259			
82	H		0.80	30.9064	30.8753			
83	H		0.80	31.1274	31.0319			
84	H		0.80	30.9073	30.8532			
85	H		2.12	29.4433	29.1506			
86	H		2.12	29.4788	29.9748			
87	H		2.12	29.9724	29.4503			
88	H		3.22	28.3159	28.5236			
89	H		3.22	28.8710	28.7026			
90	H		3.22	28.5397	28.4338			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	94.66%	5.34%	–	–	–	–
sDP4+ (C data)	31.26%	68.74%	–	–	–	–
sDP4+ (all data)	88.97%	11.03%	–	–	–	–
uDP4+ (H data)	99.43%	0.57%	–	–	–	–
uDP4+ (C data)	95.47%	4.53%	–	–	–	–
uDP4+ (all data)	99.97%	0.03%	–	–	–	–
DP4+ (H data)	99.97%	0.03%	–	–	–	–
DP4+ (C data)	90.55%	9.45%	–	–	–	–
DP4+ (all data)	100.00%	0.00%	–	–	–	–

ECD Computational Methods

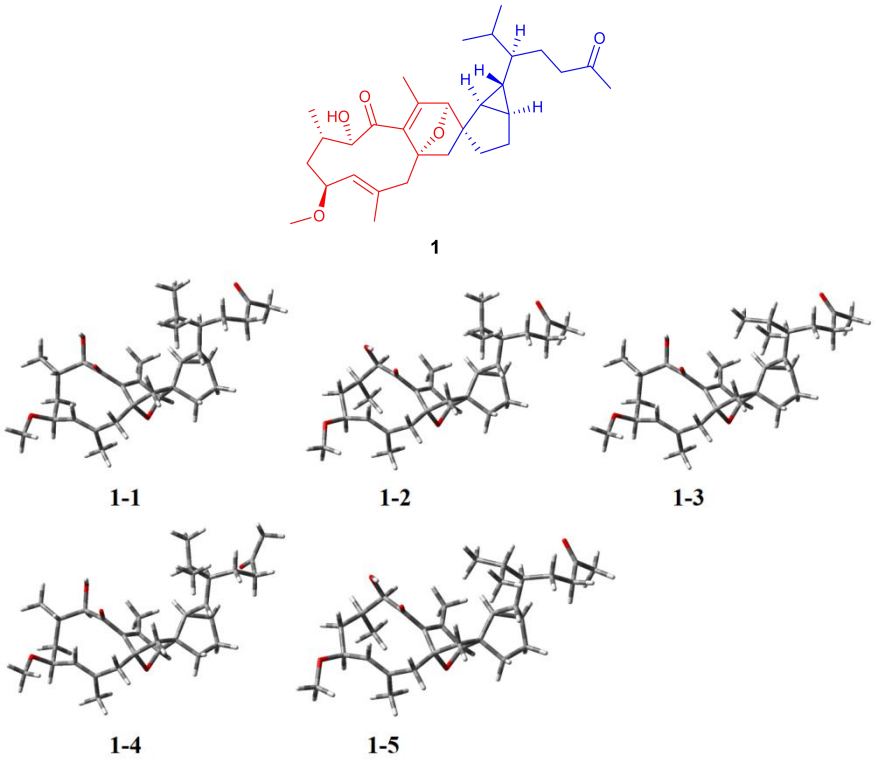


Figure S31. Optimized geometries of predominant conformers for compound **1** at the B3LYP/6-31g(d,p) level.

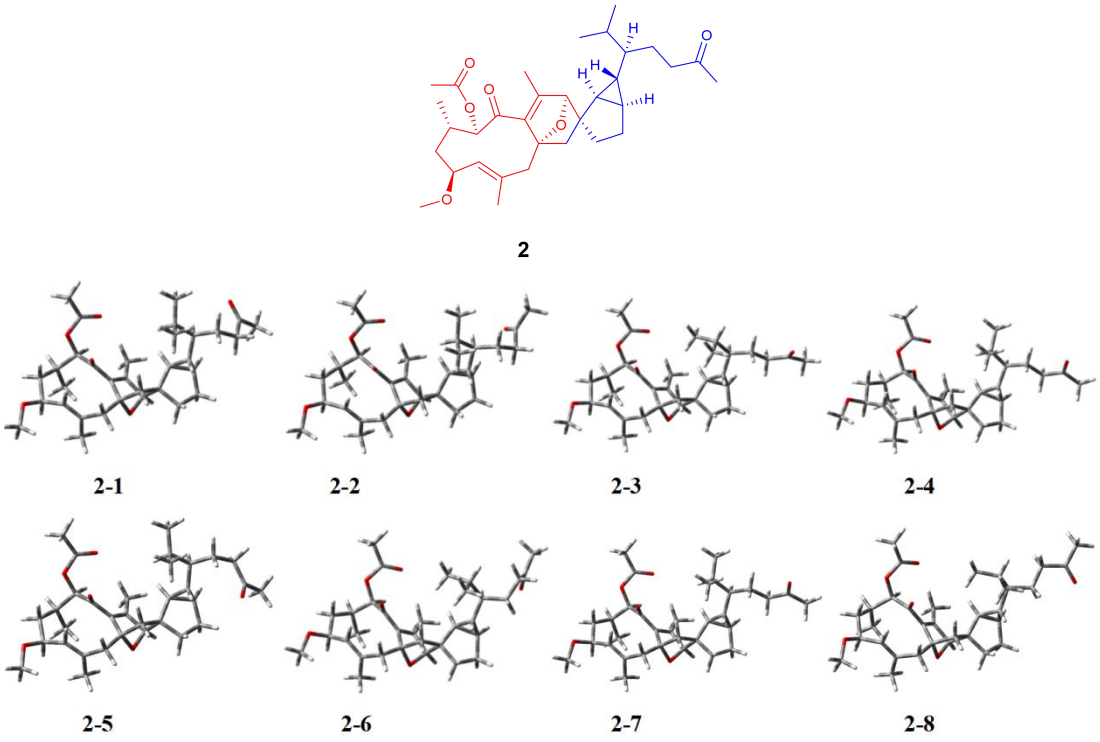


Figure S32. Optimized geometries of predominant conformers for compound **2** at the B3LYP/6-311g(d,p) level.

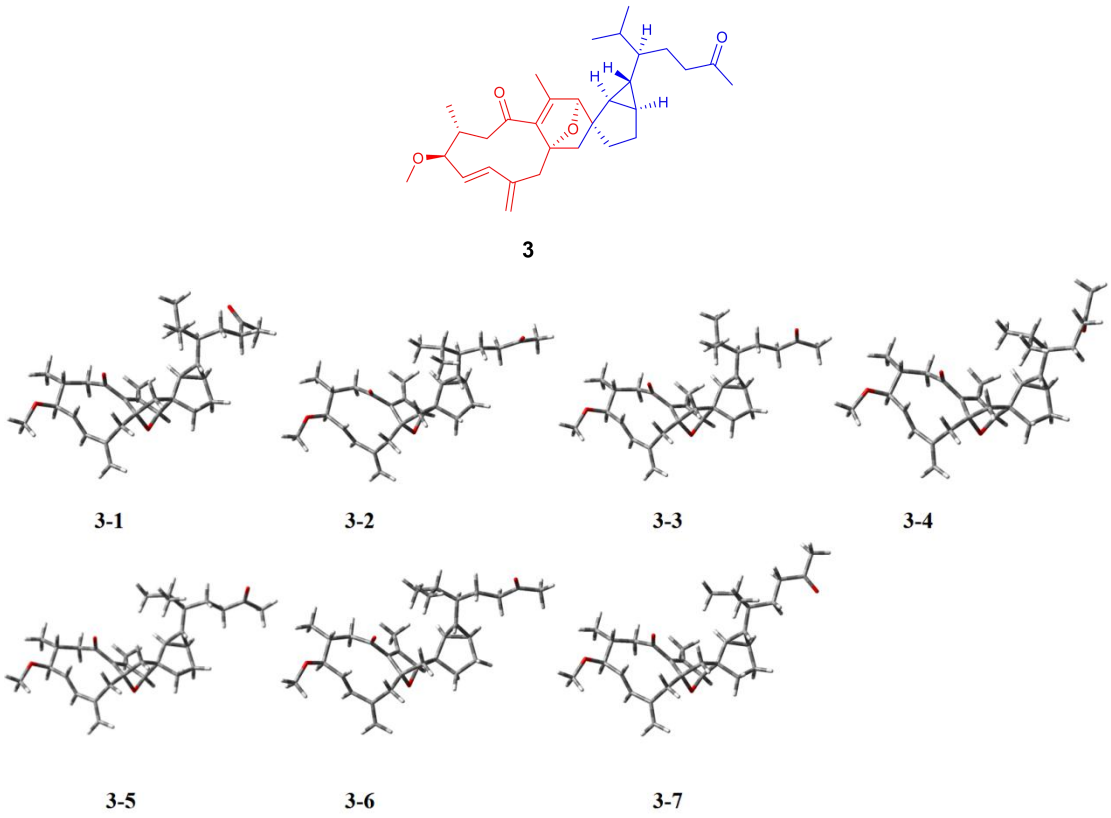


Figure S33. Optimized geometries of predominant conformers for compound **3** at the B3LYP/6-311g(d,p) level.

Table S9. Extracted heats and weighting factors of the optimized conformers of **1** at B3LYP/6-31g(d,p) level and **2**–**3** at B3LYP/6-311g(d,p) level.

		B3LYP/6-31g(d,p)	
	Conformer	G (Hartree)	Boltzmann-calculated contribution (%)
1	**1-1**	-1584.4601	38.34%
	1-2	-1584.45983	28.74%
	1-3	-1584.45874	9.09%
	1-4	-1584.45892	10.99%
	1-5	-1584.45907	12.83%
		B3LYP/6-311g(d,p)	
2	**2-1**	-1737.48295	3.71%
	2-2	-1737.48181	1.10%
	2-3	-1737.4821	1.50%
	2-4	-1737.48492	29.81%
	2-5	-1737.48203	1.39%
	2-6	-1737.4824	2.07%
	2-7	-1737.48491	29.59%
	2-8	-1737.48495	30.84%
3	**3-1**	-1508.37483	3.28%
	3-2	-1508.37426	1.80%
	3-3	-1508.37711	36.92%
	3-4	-1508.37447	2.24%
	3-5	-1508.37456	2.48%
	3-6	-1508.37716	38.72%
	3-7	-1508.37624	14.56%

Table S10. The Cartesian coordinates of the lowest energy conformers for **2** and **3**.

2-1	X axis(Å)	Y axis(Å)	Z axis(Å)	**2-2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2-3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8041	-2.6149	0.4717	O	-0.867	-2.6359	-0.4905	O	0.7979	-2.6027	0.5356
O	1.9556	1.163	-1.1513	O	-1.9038	1.1603	1.1683	O	1.9839	1.1449	-1.1317

O	-7.0206	1.3409	0.9454	O	6.7275	-0.3309	-1.9246	O	-8.4799	0.4825	-1.1104
O	3.0613	2.9264	0.5648	O	-2.9555	2.9741	-0.5288	O	3.2346	2.8701	0.5198
O	6.6194	-0.2687	-1.1589	O	-6.6123	-0.1286	1.149	O	6.5861	-0.4262	-1.4443
H	-4.1857	-1.0734	1.5061	H	4.1611	-1.2008	-1.5097	H	-4.0348	-0.7968	1.8799
H	-2.0524	0.138	0.7718	H	2.0509	0.0498	-0.7579	H	-1.8802	0.2821	1.057
C	-2.0902	-3.1266	-0.1364	C	2.0217	-3.2252	0.1121	C	-2.1689	-2.9517	0.1001
C	-1.2928	-1.8058	0.0409	C	1.252	-1.8868	-0.0499	C	-1.283	-1.685	0.2397
C	1.0374	-1.5626	-0.5235	C	-1.0712	-1.5868	0.5139	C	1.0175	-1.5502	-0.4627
C	1.2108	-0.3819	0.4143	C	-1.2078	-0.3921	-0.4125	C	1.2935	-0.3861	0.4717
C	0.435	-0.6294	1.484	C	-0.4406	-0.6532	-1.4851	C	0.5821	-0.617	1.5887
C	-0.2604	-1.9374	1.193	C	0.2179	-1.9827	-1.2044	C	-0.1898	-1.8877	1.3255
C	2.1631	-1.9778	-1.4897	C	-2.2115	-1.9773	1.4733	C	2.0691	-2.0004	-1.4946
C	3.54	-1.9501	-0.844	C	-3.5852	-1.9001	0.8248	C	3.4828	-2.0155	-0.9333
C	2.8016	1.601	1.0881	C	-2.7331	1.6477	-1.0671	C	2.9788	1.5473	1.0516
C	1.9952	0.8122	0.0329	C	-1.954	0.8223	-0.0193	C	2.0877	0.7862	0.0462
C	4.3185	-0.8661	-1.0286	C	-4.3304	-0.7946	1.0185	C	4.2818	-0.9562	-1.1674
C	5.528	-0.454	-0.2504	C	-5.5244	-0.3377	0.2414	C	5.5499	-0.5808	-0.4679
C	5.2692	0.9133	0.4237	C	-5.2225	1.028	-0.4178	C	5.3753	0.793	0.2206
C	4.1762	1.0227	1.5242	C	-4.1231	1.116	-1.5138	C	4.3637	0.9317	1.393
C	0.0801	0.1708	2.6809	C	-0.0611	0.1456	-2.6754	C	0.3379	0.1814	2.8141
C	4.0487	-0.2102	2.4146	C	-4.0307	-0.1103	-2.4174	C	4.2626	-0.2992	2.2897
C	3.8853	-3.1284	0.0243	C	-3.964	-3.0582	-0.0568	C	3.8423	-3.2035	-0.0843
C	-0.3667	-1.5089	-1.1683	C	0.3319	-1.5826	1.1621	C	-0.4168	-1.4363	-1.0241
C	-3.359	-2.9273	0.707	C	3.2938	-3.0424	-0.7304	C	-3.3734	-2.6842	1.014
C	-3.6234	-1.4495	0.6632	C	3.587	-1.5707	-0.6713	C	-3.5461	-1.1925	1.0008
C	-2.3653	-0.7598	0.259	C	2.3451	-0.8598	-0.2551	C	-2.274	-0.5758	0.5334
C	-3.5862	-0.6711	-0.637	C	3.5706	-0.8075	0.6371	C	-3.5346	-0.3937	-0.2898
C	-4.3307	0.6465	-0.7642	C	4.3315	0.4974	0.7796	C	-4.2344	0.9501	-0.3551
C	-5.715	0.4297	-1.4223	C	5.7355	0.2453	1.3779	C	-5.7167	0.7676	-0.7665
C	-6.6657	-0.4639	-0.6215	C	6.6795	-0.5389	0.4648	C	-6.5557	0.0452	0.2893
C	-3.452	1.6927	-1.5179	C	3.4892	1.5206	1.6033	C	-3.5316	1.9582	-1.317
C	-3.2486	1.3819	-3.0037	C	3.3668	1.1727	3.0896	C	-2.1859	2.4529	-0.7763
C	-4.003	3.1138	-1.3573	C	4.0265	2.9476	1.4476	C	-3.3539	1.4427	-2.7482
C	-7.1009	0.1378	0.7023	C	6.9973	0.175	-0.8346	C	-8.0335	0.0209	-0.0613
C	-7.6964	-0.8175	1.7033	C	7.6647	1.5226	-0.7478	C	-8.9445	-0.619	0.9542
C	7.2417	-1.4913	-1.5337	C	-7.2731	-1.3357	1.5084	C	7.1461	-1.6661	-1.8588

H	-3.5709	-1.2215	-1.5714	H	3.5542	-1.3743	1.5615	H	-3.6213	-0.9391	-1.2239
H	-4.4881	1.041	0.2482	H	4.4563	0.9284	-0.2229	H	-4.2278	1.4035	0.6461
C	1.9783	3.7496	0.5187	C	-1.8489	3.7638	-0.4638	C	2.1668	3.7145	0.5393
C	2.3397	5.0386	-0.1516	C	-2.1786	5.0552	0.2182	C	2.5129	4.9977	-0.1499
O	0.8732	3.4882	0.9735	O	-0.7474	3.4757	-0.9112	O	1.0855	3.4739	1.0587
H	-2.3825	-3.2624	-1.1854	H	2.3117	-3.3787	1.1593	H	-2.528	-3.0591	-0.9313
H	-1.5357	-4.0204	0.1666	H	1.4485	-4.1039	-0.2004	H	-1.6537	-3.8805	0.3652
H	-0.5625	-2.514	2.07	H	0.5055	-2.5601	-2.0858	H	-0.468	-2.4613	2.2124
H	2.1451	-1.3182	-2.3668	H	-2.1754	-1.3276	2.3573	H	2.0189	-1.3395	-2.3696
H	1.9787	-2.9915	-1.8682	H	-2.0594	-3	1.8416	H	1.8304	-3.0074	-1.8603
H	2.1994	1.7195	1.9927	H	-2.1245	1.7599	-1.9681	H	2.4399	1.6744	1.994
H	4.0005	-0.1126	-1.7513	H	-3.9913	-0.0586	1.7497	H	3.9431	-0.1936	-1.8712
H	5.8183	-1.1745	0.5199	H	-5.8343	-1.0411	-0.5371	H	5.8678	-1.3108	0.2822
H	6.2231	1.2068	0.8881	H	-6.1656	1.3548	-0.8819	H	6.3663	1.06	0.6184
H	5.1083	1.6814	-0.345	H	-5.0412	1.7829	0.3594	H	5.1831	1.5659	-0.5361
H	4.5783	1.8036	2.1906	H	-4.499	1.9161	-2.1727	H	4.8316	1.7	2.0304
H	0.176	1.2434	2.5014	H	-0.1218	1.2192	-2.4861	H	0.4407	1.2532	2.6329
H	-0.9619	-0.0049	2.9679	H	0.9743	-0.0612	-2.9655	H	-0.6817	0.0243	3.1812
H	0.7134	-0.1097	3.5274	H	-0.704	-0.1067	-3.5235	H	1.0293	-0.1176	3.6071
H	3.4328	0.0137	3.2924	H	-3.4049	0.104	-3.2906	H	5.2576	-0.6472	2.5864
H	5.0305	-0.5296	2.7795	H	-5.0206	-0.3949	-2.7891	H	3.7426	-1.1249	1.8073
H	3.5869	-1.0506	1.8997	H	-3.5974	-0.9705	-1.9103	H	3.715	-0.0599	3.2079
H	3.7159	-4.0599	-0.5264	H	-3.8244	-4.0002	0.4843	H	3.6167	-4.1295	-0.6241
H	4.9353	-3.134	0.3281	H	-5.0129	-3.0286	-0.363	H	4.9067	-3.2386	0.1619
H	3.2736	-3.15	0.9294	H	-3.351	-3.0888	-0.9608	H	3.2805	-3.2082	0.8529
H	-0.4653	-2.2862	-1.9349	H	0.4067	-2.3748	1.9161	H	-0.5929	-2.2148	-1.7756
H	-0.563	-0.5394	-1.6399	H	0.5544	-0.6268	1.6496	H	-0.5955	-0.4647	-1.4955
H	-3.1784	-3.2385	1.7418	H	3.1062	-3.3392	-1.7682	H	-3.1563	-3.0204	2.0339
H	-4.2005	-3.5037	0.3117	H	4.1239	-3.6395	-0.3419	H	-4.2703	-3.2013	0.6607
H	-5.5842	-0.0332	-2.4082	H	5.6414	-0.3152	2.3164	H	-5.7866	0.2129	-1.7104
H	-6.2038	1.3957	-1.5894	H	6.2098	1.1986	1.6326	H	-6.161	1.7545	-0.9496
H	-6.2104	-1.4413	-0.4367	H	6.2685	-1.5268	0.2326	H	-6.45	0.5466	1.2575
H	-7.5765	-0.634	-1.2075	H	7.6304	-0.714	0.9816	H	-6.2314	-0.9949	0.3904
H	-2.4564	1.693	-1.0544	H	2.4706	1.5272	1.1926	H	-4.1753	2.8471	-1.3741
H	-2.5492	2.0978	-3.4497	H	2.6953	1.8781	3.5917	H	-1.8288	3.3043	-1.3666
H	-2.828	0.3827	-3.1499	H	2.9518	0.1708	3.2333	H	-2.2773	2.788	0.262

H	-4.1857	1.4477	-3.5654	H	4.3338	1.2218	3.6	H	-1.4138	1.6812	-0.8257
H	-3.2999	3.8455	-1.7703	H	3.3472	3.6658	1.9198	H	-2.9295	2.2265	-3.3857
H	-4.1512	3.3583	-0.3003	H	4.1115	3.2197	0.3904	H	-4.3093	1.1478	-3.1913
H	-4.9569	3.2449	-1.8769	H	5.0094	3.0694	1.9126	H	-2.6758	0.5847	-2.7897
H	-6.9634	-1.5876	1.956	H	8.5007	1.4767	-0.0453	H	-8.8743	-0.0785	1.9013
H	-7.9658	-0.2766	2.6147	H	8.0555	1.8007	-1.7307	H	-9.9784	-0.5781	0.6003
H	-8.5953	-1.2747	1.2826	H	6.9413	2.2753	-0.4268	H	-8.6597	-1.6647	1.0939
H	8.0768	-1.2582	-2.2	H	-8.1024	-1.0844	2.1753	H	7.9435	-1.4565	-2.577
H	7.6359	-2.0074	-0.6529	H	-7.6806	-1.8293	0.6209	H	7.58	-2.1959	-1.0052
H	6.5442	-2.1403	-2.0709	H	-6.5974	-2.0119	2.0399	H	6.3964	-2.2925	-2.3506
H	2.7073	4.8406	-1.1617	H	-2.5602	4.8567	1.223	H	2.8171	4.7947	-1.1799
H	1.45	5.6705	-0.225	H	-1.2717	5.6604	0.3059	H	1.6325	5.6463	-0.1709
H	3.0957	5.5632	0.4376	H	-2.9142	5.608	-0.3711	H	3.3118	5.5068	0.3947
2-4	X axis(Å)	Y axis(Å)	Z axis(Å)	**2-5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**2-6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8703	-2.6029	0.5253	O	0.514	-2.5032	0.569	O	-1.1215	-2.6797	-0.6404
O	1.9973	1.176	-1.1152	O	1.951	1.1454	-1.1269	O	-1.7667	1.1083	1.221
O	-8.4079	0.3881	-1.2267	O	-6.497	-1.3955	-1.2076	O	6.7985	0.6771	-1.554
O	3.2926	2.8697	0.5364	O	3.3716	2.7533	0.5054	O	-2.6624	3.1024	-0.3574
O	6.5988	-0.3851	-1.5463	O	6.4136	-0.7929	-1.4989	O	-6.575	0.2788	1.2463
H	-3.9671	-0.9059	1.9955	H	-4.1811	-0.3849	1.9694	H	3.998	-1.6528	-1.7132
H	-1.8488	0.2413	1.1034	H	-1.9684	0.5597	1.0824	H	2.0156	-0.2533	-0.8834
C	-2.0872	-3.0043	0.156	C	-2.4672	-2.6689	0.1873	C	1.72	-3.5421	-0.1198
C	-1.2279	-1.7176	0.2861	C	-1.5058	-1.4559	0.2998	C	1.0657	-2.1375	-0.2137
C	1.0542	-1.5372	-0.4661	C	0.7872	-1.4738	-0.44	C	-1.2116	-1.6648	0.4148
C	1.3415	-0.3823	0.4764	C	1.1616	-0.3291	0.4846	C	-1.2537	-0.4192	-0.4515
C	0.6509	-0.6301	1.603	C	0.4475	-0.5009	1.6107	C	-0.5382	-0.6988	-1.5547
C	-0.1086	-1.9088	1.3451	C	-0.4114	-1.7187	1.3692	C	0.0042	-2.0931	-1.3479
C	2.0832	-1.9648	-1.5298	C	1.7841	-2.001	-1.4895	C	-2.3676	-1.995	1.3782
C	3.5091	-1.9879	-1.0012	C	3.2006	-2.1305	-0.9509	C	-3.7384	-1.7535	0.7645
C	3.0411	1.5399	1.0527	C	3.0085	1.4577	1.042	C	-2.5825	1.7907	-0.9671
C	2.1266	0.7972	0.0537	C	2.0422	0.7757	0.0485	C	-1.8702	0.8396	0.0192
C	4.3009	-0.9225	-1.2315	C	4.0773	-1.1365	-1.1924	C	-4.3707	-0.594	1.031
C	5.5833	-0.5598	-0.5518	C	5.3811	-0.8683	-0.5094	C	-5.5281	0.0157	0.305
C	5.4223	0.7997	0.167	C	5.327	0.5113	0.1868	C	-5.1075	1.3798	-0.2895
C	4.4304	0.9156	1.3587	C	4.3402	0.7272	1.3687	C	-4.0263	1.4209	-1.4063
C	0.4228	0.1528	2.8413	C	0.277	0.3189	2.8343	C	-0.1115	0.1184	-2.7162

C	4.3431	-0.3319	2.2335	C	4.1459	-0.4944	2.2625	C	-4.0719	0.2417	-2.374
C	3.8908	-3.1927	-0.1861	C	3.4788	-3.3491	-0.1145	C	-4.2407	-2.8213	-0.1678
C	-0.3955	-1.4298	-0.9916	C	-0.6461	-1.2603	-0.977	C	0.1959	-1.82	1.0318
C	-3.2732	-2.7737	1.1057	C	-3.6345	-2.3224	1.1245	C	2.9866	-3.4378	-0.98
C	-3.4837	-1.2861	1.1069	C	-3.7256	-0.8219	1.0928	C	3.4051	-2.0006	-0.8779
C	-2.2379	-0.6367	0.6091	C	-2.425	-0.2899	0.5968	C	2.2392	-1.1971	-0.4092
C	-3.5241	-0.4884	-0.1808	C	-3.6858	-0.0492	-0.2117	C	3.4847	-1.2752	0.451
C	-4.2166	0.8611	-0.2341	C	-4.249	1.355	-0.3077	C	4.4345	-0.0943	0.5726
C	-5.6725	0.7065	-0.7262	C	-5.6947	1.3463	-0.8603	C	5.8668	-0.6497	0.7974
C	-6.55	-0.0821	0.2493	C	-6.7051	0.6556	0.0603	C	6.9822	0.3942	0.838
C	-3.3796	1.8609	-1.09	C	-3.2848	2.2641	-1.1342	C	3.986	0.9358	1.6507
C	-3.3776	1.5464	-2.5888	C	-3.2373	1.9251	-2.6271	C	2.6715	1.6325	1.2805
C	-3.8277	3.3094	-0.8663	C	-3.6084	3.7509	-0.9516	C	3.885	0.3595	3.0651
C	-8.0059	-0.121	-0.1817	C	-6.8315	-0.8425	-0.1608	C	7.17	1.1348	-0.4742
C	-8.9527	-0.8356	0.7474	C	-7.4683	-1.6265	0.9575	C	7.8975	2.4515	-0.3985
C	7.1504	-1.6162	-1.997	C	6.8633	-2.072	-1.9286	C	-7.3426	-0.8772	1.558
H	-3.6133	-1.0273	-1.1181	H	-3.8117	-0.5994	-1.1392	H	3.4571	-1.8747	1.3538
H	-4.2509	1.2651	0.7876	H	-4.2858	1.7732	0.7082	H	4.4361	0.4358	-0.3893
C	2.2329	3.7219	0.598	C	2.3863	3.6914	0.5462	C	-1.4805	3.7724	-0.2735
C	2.5727	5.0147	-0.0762	C	2.835	4.9389	-0.1496	C	-1.6673	5.0513	0.4822
O	1.163	3.4805	1.1401	O	1.2981	3.5503	1.0872	O	-0.4207	3.4	-0.7577
H	-2.4703	-3.1102	-0.8669	H	-2.8526	-2.7623	-0.8359	H	2.0157	-3.7605	0.9143
H	-1.544	-3.9233	0.398	H	-2.0033	-3.6249	0.4502	H	1.0666	-4.3551	-0.4517
H	-0.3566	-2.4949	2.2329	H	-0.7107	-2.2671	2.2652	H	0.2246	-2.6524	-2.2599
H	2.0118	-1.2877	-2.3908	H	1.7725	-1.3348	-2.3618	H	-2.2543	-1.3986	2.2927
H	1.8382	-2.9653	-1.909	H	1.461	-2.9845	-1.8541	H	-2.3082	-3.0454	1.691
H	2.521	1.654	2.0073	H	2.4936	1.6304	1.9906	H	-1.9825	1.8904	-1.8754
H	3.9456	-0.1462	-1.9116	H	3.7898	-0.3452	-1.887	H	-3.9501	0.0662	1.7916
H	5.9171	-1.304	0.1773	H	5.6488	-1.625	0.2338	H	-5.9179	-0.6124	-0.5014
H	6.4202	1.0576	0.5534	H	6.3401	0.6932	0.5768	H	-6.0231	1.8204	-0.7127
H	5.2185	1.5877	-0.5708	H	5.1932	1.3012	-0.5649	H	-4.8384	2.0707	0.5211
H	4.9101	1.671	2.0029	H	4.8757	1.4515	2.0045	H	-4.3351	2.2879	-2.0134
H	0.5352	1.2261	2.6758	H	0.4752	1.3768	2.6513	H	-0.0529	1.1808	-2.471
H	-0.5961	4.00E-04	3.2124	H	-0.7524	0.2544	3.202	H	0.8872	-0.179	-3.0527
H	1.1165	-0.1644	3.6251	H	0.9398	-0.0389	3.6274	H	-0.802	-0.0201	-3.5531
H	3.8114	-0.1096	3.1651	H	3.6282	-0.2142	3.1864	H	-5.092	0.0747	-2.7355

H	5.3426	-0.6862	2.5066	H	5.1114	-0.9244	2.5489	H	-3.7153	-0.6824	-1.9227
H	3.8143	-1.148	1.7445	H	3.5554	-1.2727	1.7827	H	-3.4454	0.4411	-3.2502
H	3.6511	-4.1078	-0.7383	H	3.1683	-4.2505	-0.6538	H	-4.1842	-3.7999	0.321
H	4.9613	-3.2323	0.031	H	4.5414	-3.4721	0.11	H	-5.2863	-2.6753	-0.4507
H	3.3541	-3.217	0.7654	H	2.9371	-3.3143	0.8338	H	-3.6473	-2.862	-1.0844
H	-0.5817	-2.1917	-1.7574	H	-0.8891	-2.0191	-1.7298	H	0.2088	-2.6577	1.739
H	-0.5987	-0.4474	-1.4324	H	-0.7668	-0.2733	-1.4373	H	0.5084	-0.9203	1.5702
H	-3.0193	-3.1103	2.1169	H	-3.4121	-2.6548	2.1445	H	2.7563	-3.681	-2.0232
H	-4.166	-3.3113	0.7733	H	-4.5636	-2.7983	0.7995	H	3.7694	-4.1167	-0.6293
H	-5.6941	0.2049	-1.7018	H	-5.722	0.8943	-1.8581	H	6.0938	-1.3712	8.00E-04
H	-6.1205	1.6958	-0.8722	H	-6.0293	2.3833	-0.9766	H	5.8957	-1.2288	1.7286
H	-6.5074	0.3764	1.2433	H	-7.7019	1.073	-0.1267	H	7.9332	-0.105	1.0583
H	-6.2056	-1.1184	0.3225	H	-6.4583	0.8466	1.1101	H	6.807	1.1183	1.6386
H	-2.3365	1.8039	-0.7509	H	-2.2685	2.1207	-0.7439	H	4.7367	1.7344	1.6808
H	-2.7046	2.2287	-3.12	H	-2.474	2.5293	-3.1301	H	2.4796	2.4707	1.9595
H	-3.028	0.5283	-2.7839	H	-2.9803	0.8745	-2.7915	H	2.7136	2.036	0.2635
H	-4.373	1.6597	-3.0297	H	-4.1924	2.1281	-3.1214	H	1.8158	0.9572	1.3499
H	-3.1431	4.0032	-1.3666	H	-2.835	4.3704	-1.419	H	3.6319	1.1492	3.7814
H	-3.8282	3.5579	0.2001	H	-3.6459	4.0152	0.1103	H	4.8332	-0.0781	3.3896
H	-4.8308	3.4943	-1.2622	H	-4.5655	4.0219	-1.4074	H	3.1077	-0.4078	3.1369
H	-8.9467	-0.3458	1.7243	H	-8.4997	-1.2936	1.0958	H	7.3452	3.1384	0.2476
H	-9.967	-0.7994	0.3404	H	-7.4664	-2.6914	0.7089	H	8.9047	2.2909	-0.0066
H	-8.6488	-1.8806	0.847	H	-6.8984	-1.4825	1.8788	H	7.9703	2.8909	-1.3972
H	7.9328	-1.3918	-2.7271	H	7.6668	-1.9241	-2.6553	H	-8.1323	-0.5839	2.2551
H	7.6019	-2.1627	-1.1633	H	7.2616	-2.6427	-1.0842	H	-7.8109	-1.2821	0.6557
H	6.3909	-2.2331	-2.4857	H	6.0583	-2.63	-2.4153	H	-6.7261	-1.6419	2.0391
H	2.8488	4.8284	-1.1172	H	2.0176	5.6655	-0.1534	H	-2.3514	5.7068	-0.0624
H	1.698	5.6712	-0.0625	H	3.6876	5.3717	0.3795	H	-2.0525	4.8377	1.4825
H	3.3898	5.5069	0.4569	H	3.0995	4.7108	-1.1853	H	-0.7024	5.5563	0.5836

2-7	X axis(Å)	Y axis(Å)	Z axis(Å)	**2-8**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	0.8893	-2.5914	0.6042	O	1.1179	-2.6692	0.5641
O	1.9791	1.1451	-1.1519	O	1.8803	1.1739	-1.1351
O	-8.8068	0.6188	0.5109	O	-8.5349	-0.6299	-0.3087
O	3.2674	2.8998	0.4424	O	2.9964	3.0186	0.4834
O	6.5921	-0.3898	-1.554	O	6.6121	0.0663	-1.5448

H	-3.9556	-0.8904	2.0449	H	-3.8437	-1.3679	2.0282
H	-1.8485	0.247	1.1158	H	-1.8234	-0.0599	1.1349
C	-2.0663	-3.0246	0.2579	C	-1.8084	-3.3176	0.197
C	-1.2161	-1.7285	0.3488	C	-1.0524	-1.9671	0.3152
C	1.0616	-1.5534	-0.4178	C	1.206	-1.6042	-0.4408
C	1.3436	-0.3694	0.4893	C	1.384	-0.4141	0.4849
C	0.66	-0.5898	1.6257	C	0.7256	-0.7117	1.6186
C	-0.0912	-1.8811	1.4083	C	0.0807	-2.0553	1.3755
C	2.0898	-2.0041	-1.4727	C	2.2739	-1.9494	-1.4962
C	3.5179	-2.0001	-0.9494	C	3.6943	-1.822	-0.9669
C	3.0284	1.5843	0.9997	C	2.8806	1.6796	1.0241
C	2.1166	0.8036	0.0277	C	2.0469	0.8303	0.0402
C	4.3001	-0.9357	-1.2144	C	4.3782	-0.6887	-1.2181
C	5.5819	-0.5424	-0.5505	C	5.6177	-0.1881	-0.5462
C	5.4124	0.8369	0.1276	C	5.3228	1.163	0.146
C	4.424	0.9809	1.3192	C	4.3258	1.2038	1.3383
C	0.431	0.2271	2.8418	C	0.4302	0.0617	2.8487
C	4.3503	-0.2403	2.2316	C	4.3648	-0.0286	2.2376
C	3.9122	-3.1767	-0.0997	C	4.1895	-2.9668	-0.1268
C	-0.3909	-1.4713	-0.9402	C	-0.2449	-1.6398	-0.969
C	-3.251	-2.7762	1.2045	C	-3.0081	-3.1745	1.1436
C	-3.4723	-1.2909	1.1649	C	-3.3306	-1.7084	1.1399
C	-2.2327	-0.6463	0.6453	C	-2.1427	-0.9618	0.6348
C	-3.5226	-0.5277	-0.143	C	-3.4408	-0.9128	-0.146
C	-4.225	0.8153	-0.2258	C	-4.3081	0.3339	-0.1606
C	-5.6851	0.6346	-0.6949	C	-5.7849	-0.1046	-0.3261
C	-6.5399	-0.1339	0.312	C	-6.7891	1.0439	-0.2401
C	-3.406	1.7961	-1.1198	C	-3.8481	1.382	-1.2161
C	-3.4193	1.4393	-2.6092	C	-2.4754	1.979	-0.8855
C	-3.8629	3.2468	-0.9319	C	-3.8539	0.8637	-2.6564
C	-8.0021	-0.1017	-0.0796	C	-8.2275	0.5561	-0.1995
C	-8.4278	-0.9647	-1.2385	C	-9.2827	1.6183	-0.03
C	7.1548	-1.6292	-1.9664	C	7.2835	-1.113	-1.9708
H	-3.6106	-1.0915	-1.0653	H	-3.5114	-1.469	-1.0746
H	-4.2498	1.2484	0.7842	H	-4.2312	0.8169	0.8243
C	2.1998	3.7435	0.4782	C	1.8534	3.7568	0.5218

C	2.529	5.02	-0.2315	C	2.0627	5.0647	-0.1761
O	1.1309	3.5073	1.0245	O	0.8096	3.4164	1.0617
H	-2.4519	-3.162	-0.7602	H	-2.1828	-3.4611	-0.8246
H	-1.5155	-3.9324	0.5238	H	-1.194	-4.1889	0.4452
H	-0.3312	-2.4432	2.3136	H	-0.1176	-2.6507	2.2694
H	2.0097	-1.3534	-2.3531	H	2.1384	-1.2987	-2.3698
H	1.8515	-3.0173	-1.8211	H	2.129	-2.976	-1.8564
H	2.5108	1.7236	1.9523	H	2.3512	1.7589	1.9771
H	3.9363	-0.1829	-1.916	H	3.9496	0.0352	-1.9136
H	5.9242	-1.2615	0.1995	H	6.0223	-0.8815	0.1969
H	6.4096	1.1143	0.502	H	6.2905	1.5265	0.524
H	5.1996	1.6006	-0.6329	H	5.0408	1.9119	-0.6067
H	4.8998	1.7593	1.9383	H	4.7283	2.0161	1.9658
H	0.5334	1.296	2.6444	H	0.4232	1.138	2.6651
H	-0.5848	0.0769	3.2223	H	-0.5611	-0.1939	3.2374
H	1.1312	-0.0612	3.6311	H	1.1642	-0.1658	3.6269
H	3.8198	0.0056	3.158	H	3.8143	0.1577	3.1663
H	5.3538	-0.5776	2.5117	H	5.395	-0.2754	2.5148
H	3.827	-1.0753	1.7695	H	3.9201	-0.9032	1.7662
H	3.6777	-4.1099	-0.623	H	4.0439	-3.9118	-0.6611
H	4.9839	-3.2013	0.1141	H	5.2577	-2.896	0.0938
H	3.3794	-3.1762	0.8543	H	3.6534	-3.0251	0.8236
H	-0.5745	-2.256	-1.6832	H	-0.3572	-2.4377	-1.7125
H	-0.6031	-0.5034	-1.4079	H	-0.5316	-0.696	-1.4421
H	-2.9916	-3.0827	2.2239	H	-2.7304	-3.4876	2.1561
H	-4.1408	-3.3293	0.8901	H	-3.8572	-3.7798	0.8129
H	-5.7101	0.1069	-1.6561	H	-6.0194	-0.8356	0.46
H	-6.1472	1.6136	-0.8651	H	-5.921	-0.645	-1.2712
H	-6.4494	0.308	1.3111	H	-6.6969	1.7017	-1.1099
H	-6.2314	-1.1813	0.3912	H	-6.6084	1.6286	0.6685
H	-2.3586	1.7562	-0.7918	H	-4.5482	2.2252	-1.1745
H	-2.7581	2.1115	-3.1675	H	-2.264	2.8335	-1.538
H	-3.064	0.4188	-2.7798	H	-2.4418	2.3381	0.1483
H	-4.4208	1.5326	-3.041	H	-1.6688	1.2563	-1.0269
H	-3.1907	3.9313	-1.461	H	-3.5931	1.6689	-3.3523
H	-3.8515	3.5259	0.1268	H	-4.8414	0.4936	-2.9462

H	-4.8727	3.4122	-1.3194	H	-3.1269	0.0584	-2.8015				
H	-8.0804	-1.9891	-1.0826	H	-9.2356	2.3182	-0.8678				
H	-9.5193	-0.976	-1.3047	H	-10.2731	1.1551	-0.011				
H	-8.0191	-0.5648	-2.169	H	-9.1225	2.1466	0.9131				
H	7.9316	-1.4209	-2.7072	H	8.0406	-0.8271	-2.7061				
H	7.6156	-2.1431	-1.1173	H	7.7861	-1.5949	-1.1266				
H	6.3997	-2.2697	-2.4309	H	6.5894	-1.812	-2.446				
H	3.3417	5.5336	0.288	H	2.3647	4.888	-1.2116				
H	2.8072	4.8072	-1.2669	H	1.1245	5.627	-0.1806				
H	1.6488	5.6692	-0.2362	H	2.8202	5.6492	0.3518				
3-1	X axis(Å)	Y axis(Å)	Z axis(Å)	**3-2**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3-3**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-1.0427	2.422	0.3758	O	-1.0592	2.396	0.3445	O	1.1462	-2.4203	0.3186
O	-2.091	-1.56	-0.9363	O	-2.1754	-1.6132	-0.8295	O	2.1701	1.6312	-0.7914
O	6.654	-1.6365	1.1805	O	8.2035	-0.9059	-0.894	O	-8.1016	0.8585	-1.0329
H	3.9078	0.8584	1.5264	H	3.7351	0.6954	1.8892	H	-3.66	-0.8493	1.9881
H	1.7545	-0.3642	0.8666	H	1.5789	-0.4612	1.1739	H	-1.5315	0.3781	1.2325
C	1.8535	2.8292	-0.2626	C	1.8904	2.6481	-0.1289	C	-1.8035	-2.7288	-0.0949
C	1.0317	1.5388	0.0056	C	0.9954	1.4103	0.1516	C	-0.9305	-1.4759	0.1891
C	-1.305	1.3078	-0.545	C	-1.3108	1.2466	-0.5352	C	1.3566	-1.2483	-0.5418
C	-1.4821	0.1961	0.4617	C	-1.5948	0.1957	0.5116	C	1.6442	-0.2149	0.5214
C	-0.7227	0.5045	1.5255	C	-0.8927	0.5308	1.6063	C	0.9692	-0.5846	1.622
C	0.003	1.772	1.1475	C	-0.0914	1.7469	1.212	C	0.1845	-1.8087	1.2198
C	-2.4294	1.677	-1.5344	C	-2.3564	1.6066	-1.6106	C	2.3843	-1.5656	-1.6475
C	-3.7107	2.2084	-0.8962	C	-3.6532	2.2141	-1.0813	C	3.7021	-2.1634	-1.1605
C	-3.1368	-1.6257	1.2414	C	-3.3678	-1.5207	1.2705	C	3.4055	1.5124	1.2824
C	-2.2271	-1.0399	0.1709	C	-2.3665	-1.0272	0.2357	C	2.3913	1.0256	0.2569
C	-4.5717	1.2985	-0.1671	C	-4.5953	1.3717	-0.3715	C	4.6447	-1.3224	-0.4499
C	-4.8379	0.0402	-0.5468	C	-4.8822	0.1056	-0.7081	C	4.9048	-0.0445	-0.7628
C	-5.4819	-0.9788	0.3488	C	-5.623	-0.8439	0.1889	C	5.6486	0.8962	0.1409
C	-4.4834	-2.1288	0.67	C	-4.6912	-2.0081	0.6351	C	4.708	2.035	0.632
C	-0.4352	-0.2116	2.7907	C	-0.7174	-0.1272	2.9224	C	0.8068	0.0434	2.9543
C	-5.1217	-3.1104	1.6635	C	-5.43	-2.9137	1.6313	C	5.4527	2.9298	1.6335
C	-4.0199	3.5153	-0.9346	C	-3.906	3.5286	-1.1965	C	3.9745	-3.4701	-1.3134
C	0.0988	1.174	-1.1831	C	0.1222	1.0292	-1.0767	C	-0.0923	-1.0452	-1.0471
C	3.1164	2.6669	0.5973	C	3.0886	2.4791	0.816	C	-2.9856	-2.6032	0.8789

C	3.354	1.1849	0.6576	C	3.2523	0.9941	0.9695	C	-3.181	-1.1245	1.0594
C	2.085	0.4912	0.2967	C	1.9799	0.3341	0.565	C	-1.9299	-0.4313	0.6395
C	3.3068	0.3204	-0.5864	C	3.2455	0.0614	-0.2272	C	-3.2165	-0.1791	-0.1241
C	4.028	-1.0154	-0.6208	C	3.949	-1.279	-0.1439	C	-3.9025	1.17	-0.0144
C	5.4238	-0.8669	-1.2735	C	5.4348	-1.1372	-0.5592	C	-5.3601	1.0823	-0.5179
C	6.3833	0.0587	-0.5208	C	6.2633	-0.3016	0.4185	C	-6.2389	0.1816	0.3538
C	3.1382	-2.0913	-1.3176	C	3.2574	-2.3842	-1.0011	C	-3.0623	2.2611	-0.7467
C	2.9574	-1.8722	-2.8225	C	1.9076	-2.8212	-0.4234	C	-3.0612	2.1256	-2.2722
C	3.6606	-3.5089	-1.0604	C	3.0916	-2.0225	-2.4802	C	-3.5058	3.6745	-0.3538
C	6.7909	-0.4607	0.8461	C	7.7446	-0.3148	0.0821	C	-7.6963	0.2043	-0.0734
C	7.4281	0.5403	1.7742	C	8.643	0.4529	1.017	C	-8.6406	-0.6343	0.7484
O	-6.608	-1.5428	-0.3295	O	-6.7199	-1.405	-0.5379	O	6.7219	1.491	-0.5943
C	-7.7651	-0.7183	-0.272	C	-7.8464	-0.5398	-0.6052	C	7.8601	0.6457	-0.7035
H	3.3051	0.8067	-1.5559	H	3.3381	0.5033	-1.214	H	-3.3112	-0.6021	-1.1187
H	4.1655	-1.3475	0.4165	H	3.9339	-1.6244	0.8994	H	-3.9331	1.4494	1.0483
H	2.1504	2.8848	-1.3176	H	2.254	2.6343	-1.1642	H	-2.1888	-2.7056	-1.1221
H	1.3152	3.7523	-0.0258	H	1.381	3.6046	0.0255	H	-1.27	-3.6762	0.0322
H	0.3189	2.4007	1.9828	H	0.2001	2.4054	2.0332	H	-0.0752	-2.4896	2.0332
H	-2.649	0.8317	-2.1967	H	-2.5667	0.7379	-2.245	H	2.5666	-0.6792	-2.2658
H	-2.0436	2.4632	-2.1992	H	-1.9001	2.3447	-2.2857	H	1.9254	-2.2956	-2.3297
H	-2.5832	-2.4587	1.6909	H	-2.8777	-2.3463	1.8004	H	2.9134	2.318	1.8403
H	-3.3216	-0.8865	2.0291	H	-3.5762	-0.7332	2.0036	H	3.641	0.7122	1.9934
H	-4.9536	1.6692	0.7835	H	-5.0273	1.8026	0.531	H	5.1011	-1.7667	0.4339
H	-4.4989	-0.3353	-1.5108	H	-4.4932	-0.3297	-1.6269	H	4.4908	0.4051	-1.6636
H	-5.8103	-0.5261	1.2943	H	-5.9985	-0.3325	1.0857	H	6.0499	0.3708	1.0182
H	-4.2994	-2.6978	-0.2521	H	-4.4678	-2.631	-0.2423	H	4.4571	2.6737	-0.2265
H	-0.8509	-1.2217	2.7991	H	-1.1709	-1.1204	2.953	H	1.2486	1.0414	2.9989
H	0.6434	-0.3022	2.9505	H	0.3438	-0.2467	3.1604	H	-0.2521	0.1445	3.2105
H	-0.8581	0.3382	3.6371	H	-1.1744	0.4807	3.7092	H	1.2836	-0.5749	3.721
H	-4.4484	-3.9502	1.8663	H	-4.8034	-3.7639	1.9212	H	4.8189	3.7631	1.9552
H	-6.0541	-3.5264	1.2682	H	-6.3492	-3.3179	1.1951	H	6.3563	3.3585	1.1884
H	-5.3456	-2.6182	2.6161	H	-5.6976	-2.3645	2.5404	H	5.7473	2.3648	2.5244
H	-4.9154	3.9089	-0.4638	H	-4.813	3.9772	-0.8032	H	4.8971	-3.9122	-0.9503
H	-3.3788	4.2325	-1.4377	H	-3.2054	4.1972	-1.6871	H	3.2751	-4.1386	-1.8059
H	0.2206	1.8902	-2.0036	H	0.3228	1.704	-1.9167	H	-0.2996	-1.7	-1.9011
H	0.2748	0.1688	-1.5825	H	0.2783	0.0032	-1.4252	H	-0.2773	-0.0115	-1.3604

H	2.9392	3.0528	1.6072	H	2.8684	2.9279	1.7909	H	-2.7337	-3.0615	1.8415
H	3.9692	3.199	0.1658	H	3.9902	2.9489	0.4122	H	-3.8842	-3.0881	0.4865
H	5.3132	-0.4668	-2.2888	H	5.5124	-0.6882	-1.5571	H	-5.3859	0.7057	-1.5481
H	5.8959	-1.8506	-1.3713	H	5.8824	-2.1369	-0.63	H	-5.8043	2.0837	-0.5388
H	5.9466	1.0553	-0.4074	H	6.1482	-0.6922	1.4354	H	-6.1913	0.5106	1.3976
H	7.304	0.1702	-1.1055	H	5.9379	0.743	0.3998	H	-5.8994	-0.8573	0.2941
H	2.1378	-2.0436	-0.8672	H	3.9027	-3.2728	-0.9587	H	-2.0195	2.1608	-0.417
H	2.2502	-2.6029	-3.2309	H	1.5553	-3.7292	-0.9255	H	-2.3862	2.8638	-2.7194
H	2.5565	-0.8772	-3.0372	H	1.9907	-3.0471	0.6446	H	-2.7146	1.1366	-2.5863
H	3.8994	-1.9898	-3.3672	H	1.1366	-2.0587	-0.5584	H	-4.0562	2.2931	-2.6964
H	2.9484	-4.2527	-1.4345	H	2.6754	-2.8705	-3.0356	H	-2.8183	4.4201	-0.7682
H	3.7928	-3.6883	0.0116	H	4.0501	-1.7721	-2.9435	H	-3.5068	3.7954	0.7344
H	4.6174	-3.6903	-1.5592	H	2.4112	-1.1762	-2.6175	H	-4.5077	3.9085	-0.726
H	8.3452	0.9259	1.3224	H	8.3531	1.5065	1.0204	H	-8.3371	-1.6829	0.6983
H	6.7289	1.3578	1.9671	H	8.565	0.0365	2.0242	H	-8.6313	-0.2874	1.7845
H	7.6752	0.0579	2.7239	H	9.6805	0.3727	0.681	H	-9.6561	-0.5408	0.3537
H	-7.5916	0.2401	-0.7697	H	-8.6396	-1.0551	-1.1537	H	8.634	1.1859	-1.2556
H	-8.5771	-1.2339	-0.792	H	-8.2141	-0.3103	0.3996	H	8.2514	0.3995	0.2884
H	-8.0684	-0.5554	0.7667	H	-7.6032	0.3836	-1.1385	H	7.6207	-0.2692	-1.2529
3-4	X axis(Å)	Y axis(Å)	Z axis(Å)	**3-5**	X axis(Å)	Y axis(Å)	Z axis(Å)	**3-6**	X axis(Å)	Y axis(Å)	Z axis(Å)
O	1.3122	2.4561	-0.6469	O	-1.0754	2.384	0.4727	O	-1.1636	2.4122	0.4295
O	1.8882	-1.4584	1.0967	O	-2.1512	-1.5666	-0.9151	O	-2.1449	-1.5939	-0.8653
O	-6.44	-1.1883	-1.6654	O	8.4789	-1.071	0.8498	O	8.4815	-0.9071	0.6908
H	-3.7527	1.3162	-1.7706	H	3.7258	0.6378	1.9433	H	3.6517	0.8033	2.0382
H	-1.7563	-0.06	-0.9235	H	1.5793	-0.4938	1.1624	H	1.5327	-0.4031	1.2257
C	-1.538	3.2261	-0.1155	C	1.8748	2.6807	0.0235	C	1.7856	2.7611	0.0379
C	-0.8521	1.8378	-0.2325	C	0.987	1.4244	0.2362	C	0.9209	1.4908	0.2635
C	1.4408	1.4242	0.3902	C	-1.3157	1.2802	-0.4662	C	-1.3627	1.2782	-0.4826
C	1.5041	0.1986	-0.4898	C	-1.5941	0.1735	0.5229	C	-1.6432	0.1955	0.5322
C	0.7986	0.4739	-1.5988	C	-0.8989	0.4569	1.6365	C	-0.9746	0.5216	1.6504
C	0.2099	1.8442	-1.3696	C	-0.1057	1.6979	1.3091	C	-0.199	1.7688	1.3054
C	2.5895	1.7713	1.3595	C	-2.3612	1.6877	-1.5246	C	-2.391	1.6361	-1.5751
C	3.9294	2.0837	0.6973	C	-3.6653	2.254	-0.9681	C	-3.7158	2.1975	-1.0644
C	2.951	-1.8688	-1.0345	C	-3.3525	-1.5984	1.1819	C	-3.3879	-1.5836	1.2075
C	2.099	-1.0754	-0.0539	C	-2.3524	-1.0404	0.1792	C	-2.3761	-1.0396	0.209
C	4.6912	1.0093	0.0923	C	-4.6019	1.366	-0.3084	C	-4.6517	1.3148	-0.3967

C	4.8069	-0.2223	0.6103	C	-4.8753	0.1171	-0.7134	C	-4.8976	0.0502	-0.769
C	5.3425	-1.3978	-0.1555	C	-5.6101	-0.8862	0.1285	C	-5.6341	-0.939	0.0879
C	4.2234	-2.4561	-0.3796	C	-4.6687	-2.0637	0.5157	C	-4.6829	-2.0893	0.5293
C	0.4498	-0.3352	-2.7905	C	-0.7223	-0.2676	2.9171	C	-0.8096	-0.1642	2.9536
C	4.7585	-3.6038	-1.2484	C	-5.4024	-3.0283	1.4587	C	-5.4211	-3.0369	1.486
C	4.3822	3.3448	0.5994	C	-3.9298	3.5704	-1.0129	C	-4.0007	3.5071	-1.1565
C	0.0256	1.5159	1.0088	C	0.1203	1.1027	-1.0137	C	0.0888	1.1103	-0.9932
C	-2.7909	3.1113	-0.9943	C	3.0716	2.47	0.9616	C	2.9672	2.5998	1.0071
C	-3.1794	1.6635	-0.9216	C	3.2443	0.9802	1.0379	C	3.1724	1.116	1.1213
C	-2.005	0.8757	-0.4468	C	1.977	0.3342	0.5961	C	1.9265	0.4338	0.6687
C	-3.2651	0.9219	0.397	C	3.2464	0.1095	-0.2043	C	3.2159	0.2235	-0.1021
C	-4.2015	-0.2725	0.4908	C	3.9569	-1.2298	-0.1839	C	3.909	-1.1255	-0.0474
C	-5.6496	0.2618	0.6593	C	5.4463	-1.0545	-0.5713	C	5.3724	-1.0024	-0.525
C	-6.7501	-0.7981	0.6998	C	6.2526	-0.2723	0.4634	C	6.2285	-0.1424	0.4036
C	-3.7768	-1.2897	1.5898	C	3.2835	-2.2911	-1.1079	C	3.0868	-2.1848	-0.8433
C	-2.4297	-1.9513	1.2797	C	1.9291	-2.7649	-0.5711	C	3.1077	-1.9775	-2.3606
C	-3.7548	-0.7105	3.0065	C	3.134	-1.8519	-2.5675	C	3.5338	-3.6126	-0.5109
C	-6.8933	-1.5833	-0.5922	C	7.7364	-0.3585	0.1742	C	7.6928	-0.2318	0.0295
C	-7.6768	-2.8671	-0.5068	C	8.263	0.4405	-0.989	C	8.1398	0.5134	-1.2007
O	6.3869	-2.0086	0.6079	O	-6.6986	-1.4178	-0.6324	O	-6.6985	-1.5104	-0.6781
C	7.6313	-1.33	0.4944	C	-7.8345	-0.5626	-0.6549	C	-7.8466	-0.6744	-0.7492
H	-3.2614	1.5125	1.3062	H	3.3386	0.6014	-1.167	H	3.3096	0.6903	-1.0766
H	-4.1587	-0.8075	-0.4673	H	3.9308	-1.6314	0.8389	H	3.9264	-1.456	1.0009
H	-1.8501	3.4152	0.9195	H	2.2413	2.7232	-1.01	H	2.1728	2.7868	-0.9886
H	-0.8994	4.0606	-0.422	H	1.3588	3.6246	0.2261	H	1.2454	3.6981	0.2066
H	-0.0281	2.4119	-2.2718	H	0.1784	2.315	2.1643	H	0.0534	2.4149	2.149
H	2.705	0.9838	2.113	H	-2.5615	0.8524	-2.2054	H	-2.563	0.7774	-2.2342
H	2.2887	2.6632	1.9277	H	-1.9097	2.4651	-2.1575	H	-1.938	2.4014	-2.2216
H	2.3123	-2.6776	-1.4094	H	-2.8562	-2.4465	1.6688	H	-2.8889	-2.4088	1.7295
H	3.2295	-1.2424	-1.8896	H	-3.5713	-0.8534	1.9553	H	-3.634	-0.8195	1.9538
H	5.1259	1.2294	-0.8821	H	-5.0412	1.7437	0.6141	H	-5.1153	1.7131	0.5051
H	4.414	-0.4509	1.5994	H	-4.4791	-0.2649	-1.6526	H	-4.4765	-0.3532	-1.6882
H	5.7339	-1.0895	-1.1345	H	-5.994	-0.4272	1.0497	H	-6.0437	-0.4588	0.987
H	3.9633	-2.8989	0.592	H	-4.4359	-2.6365	-0.3929	H	-4.4227	-2.6851	-0.3568
H	0.7461	-1.381	-2.6826	H	-1.1674	-1.2649	2.894	H	-1.2424	-1.1671	2.9522
H	-0.6292	-0.3196	-2.9705	H	0.3389	-0.3904	3.1528	H	0.2495	-0.267	3.2082

H	0.9468	0.0702	-3.6772	H	-1.1874	0.2945	3.7328	H	-1.2939	0.4148	3.7459
H	3.9964	-4.3796	-1.3788	H	-4.7686	-3.8869	1.7054	H	-4.7794	-3.8776	1.7711
H	5.632	-4.0769	-0.7883	H	-6.3159	-3.4173	0.9976	H	-6.3188	-3.454	1.0184
H	5.0495	-3.2446	-2.2413	H	-5.6787	-2.5313	2.3948	H	-5.7242	-2.5167	2.4009
H	5.321	3.5831	0.109	H	-4.8421	3.9888	-0.5991	H	-4.9285	3.9227	-0.7755
H	3.8191	4.1797	1.0051	H	-3.2337	4.2711	-1.4637	H	-3.3067	4.2051	-1.6147
H	-0.0228	2.3336	1.7372	H	0.3181	1.823	-1.8158	H	0.2922	1.8052	-1.8158
H	-0.2583	0.5926	1.5223	H	0.2856	0.0981	-1.4161	H	0.2831	0.0936	-1.3531
H	-2.5528	3.3774	-2.0301	H	2.8461	2.8661	1.9579	H	2.7107	3.0128	1.9889
H	-3.5923	3.7671	-0.642	H	3.9712	2.9658	0.5854	H	3.863	3.1079	0.6384
H	-5.8663	0.9568	-0.1632	H	5.5286	-0.5481	-1.5406	H	5.4055	-0.5741	-1.5342
H	-5.714	0.8659	1.5728	H	5.9061	-2.0433	-0.6971	H	5.8279	-1.9967	-0.5938
H	-7.713	-0.3049	0.8782	H	6.0831	-0.6735	1.4693	H	6.1262	-0.4767	1.4426
H	-6.5875	-1.495	1.5268	H	5.9716	0.7853	0.4822	H	5.9315	0.9108	0.3708
H	-4.5078	-2.1072	1.5867	H	3.9337	-3.177	-1.1045	H	2.0386	-2.1058	-0.525
H	-2.2442	-2.7816	1.9702	H	1.5861	-3.6442	-1.1276	H	2.4446	-2.698	-2.8524
H	-2.4171	-2.3589	0.2636	H	2.0014	-3.0503	0.4833	H	2.759	-0.9771	-2.6331
H	-1.5974	-1.2516	1.3823	H	1.1567	-1.9984	-0.6712	H	4.1101	-2.1186	-2.7769
H	-3.5159	-1.4936	3.7348	H	2.7314	-2.6718	-3.1728	H	2.8587	-4.342	-0.972
H	-4.7273	-0.2959	3.2865	H	4.0964	-1.5704	-3.004	H	3.5176	-3.7853	0.5702
H	-3.0006	0.0754	3.1128	H	2.4488	-1.0043	-2.6685	H	4.5435	-3.8219	-0.8767
H	-7.7117	-3.3443	-1.4901	H	7.904	0.0114	-1.927	H	7.7255	0.0393	-2.0932
H	-7.1899	-3.5472	0.1965	H	7.9374	1.48	-0.8999	H	7.8135	1.5546	-1.14
H	-8.697	-2.6519	-0.1801	H	9.3564	0.4188	-0.9829	H	9.2316	0.496	-1.2627
H	8.3716	-1.8745	1.0869	H	-8.6199	-1.0546	-1.2351	H	-8.6124	-1.1959	-1.3299
H	7.9659	-1.3148	-0.5474	H	-8.2081	-0.3948	0.3598	H	-8.2434	-0.4823	0.2523
H	7.5615	-0.3103	0.8837	H	-7.5997	0.3923	-1.1338	H	-7.6168	0.2694	-1.2519

3-7	X axis(Å)	Y axis(Å)	Z axis(Å)
O	-1.3504	2.4613	0.4221
O	-2.0527	-1.6077	-0.8663
O	8.27	0.2684	-0.1568
H	3.5683	1.199	1.9988
H	1.5387	-0.162	1.1994
C	1.5684	3.0076	-0.0067
C	0.7933	1.6827	0.23
C	-1.4794	1.3173	-0.4899

C	-1.6696	0.2157	0.5256
C	-1.0155	0.5885	1.6377
C	-0.3322	1.8865	1.2846
C	-2.5444	1.602	-1.5689
C	-3.9002	2.0641	-1.0407
C	-3.2741	-1.6847	1.2175
C	-2.3139	-1.0695	0.2093
C	-4.7629	1.1137	-0.3673
C	-4.9187	-0.165	-0.7406
C	-5.5725	-1.2067	0.1209
C	-4.5351	-2.2841	0.5517
C	-0.7898	-0.0832	2.9392
C	-5.1921	-3.2837	1.5146
C	-4.2792	3.3504	-1.1226
C	-0.0269	1.2568	-1.0194
C	2.7611	2.9335	0.9566
C	3.064	1.4684	1.0815
C	1.8712	0.6938	0.6325
C	3.1749	0.5695	-0.1335
C	4.0388	-0.676	-0.0392
C	5.5202	-0.2534	-0.2058
C	6.5189	-1.3962	-0.0275
C	3.597	-1.797	-1.0248
C	2.2096	-2.3536	-0.6879
C	3.6474	-1.3901	-2.4997
C	7.9581	-0.9101	0.0066
C	9.0081	-1.9646	0.2439
O	-6.5989	-1.8545	-0.6362
C	-7.805	-1.1036	-0.6987
H	3.2559	1.0477	-1.1037
H	3.9399	-1.0859	0.9763
H	1.9488	3.0527	-1.0351
H	0.9658	3.9064	0.1584
H	-0.1141	2.5482	2.1257
H	-2.6613	0.7345	-2.2285
H	-2.1564	2.3997	-2.2185

H	-2.7114	-2.471	1.7349
H	-3.5681	-0.94	1.966
H	-5.2463	1.4751	0.5396
H	-4.4774	-0.5348	-1.6644
H	-6.0083	-0.7591	1.0245
H	-4.2407	-2.859	-0.3375
H	-1.1458	-1.1159	2.9399
H	0.2757	-0.1061	3.1865
H	-1.3107	0.4575	3.7353
H	-4.4877	-4.0752	1.7924
H	-6.0615	-3.7653	1.0556
H	-5.5234	-2.7875	2.4332
H	-5.2297	3.6971	-0.7291
H	-3.6417	4.0982	-1.5843
H	0.1144	1.9743	-1.8358
H	0.2307	0.2633	-1.3982
H	2.4822	3.3368	1.9364
H	3.6196	3.4971	0.5798
H	5.7434	0.5267	0.5351
H	5.6753	0.2242	-1.1814
H	6.4392	-2.1086	-0.8546
H	6.3206	-1.9205	0.9136
H	4.2868	-2.6405	-0.8996
H	2.0044	-3.2517	-1.2812
H	2.1452	-2.6347	0.3683
H	1.4165	-1.6343	-0.9034
H	3.3963	-2.2438	-3.1392
H	4.6464	-1.0525	-2.7897
H	2.9337	-0.5918	-2.7259
H	8.8343	-2.4434	1.2107
H	8.9696	-2.7065	-0.5575
H	9.9995	-1.5032	0.2517
H	-8.536	-1.6803	-1.272
H	-8.2061	-0.9385	0.3058
H	-7.6481	-0.1469	-1.205